

AD-A202 262

DTIC FILE COPY

DTIC = 0
ADR 188571
ESL-TR-86-66
VOL II
1

EVALUATION AND PREDICTION OF
HENRY'S LAW CONSTANTS AND
AQUEOUS SOLUBILITIES FOR
SOLVENTS AND HYDROCARBON FUEL
COMPONENTS
VOL II: EXPERIMENTAL HENRY'S LAW
DATA

G.B. HOWE, M.E. MULLINS, T.N. ROGERS

RESEARCH TRIANGLE INSTITUTE
P.O. BOX 12194
RESEARCH TRIANGLE PARK NC 27709

SEPTEMBER 1987

FINAL REPORT

FEBRUARY 1985 - SEPTEMBER 1986

DTIC
ELECTED
DEC 12 1988

APPROVED FOR PUBLIC RELEASE: DISTRIBUTION UNLIMITED



ENGINEERING & SERVICES LABORATORY
AIR FORCE ENGINEERING & SERVICES CENTER
TYNDALL AIR FORCE BASE, FLORIDA 32403

88 12 9 055

NOTICE

PLEASE DO NOT REQUEST COPIES OF THIS REPORT FROM
HQ AFESC/RD (ENGINEERING AND SERVICES LABORATORY).
ADDITIONAL COPIES MAY BE PURCHASED FROM:

NATIONAL TECHNICAL INFORMATION SERVICE
5285 PORT ROYAL ROAD
SPRINGFIELD, VIRGINIA 22161

FEDERAL GOVERNMENT AGENCIES AND THEIR CONTRACTORS
REGISTERED WITH DEFENSE TECHNICAL INFORMATION CENTER
SHOULD DIRECT REQUESTS FOR COPIES OF THIS REPORT TO:

DEFENSE TECHNICAL INFORMATION CENTER
CAMERON STATION
ALEXANDRIA, VIRGINIA 22314

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

Form Approved
OMB No. 0704-0188

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b. RESTRICTIVE MARKINGS N/A										
2a. SECURITY CLASSIFICATION AUTHORITY N/A		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release. Distribution Unlimited										
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE N/A		5. MONITORING ORGANIZATION REPORT NUMBER(S) ESL-86-66										
4. PERFORMING ORGANIZATION REPORT NUMBER(S)		7a. NAME OF MONITORING ORGANIZATION HQ AFESC/RDVW										
6a. NAME OF PERFORMING ORGANIZATION Research Triangle Institute	6b. OFFICE SYMBOL (If applicable)	7b. ADDRESS (City, State, and ZIP Code) Tyndall AFB FL 32403										
6c. ADDRESS (City, State, and ZIP Code) P.O. Box 12194 Research Triangle Park NC 27709		8a. NAME OF FUNDING / SPONSORING ORGANIZATION Same as Block 7										
8c. ADDRESS (City, State, and ZIP Code)		8b. OFFICE SYMBOL (If applicable)										
		9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F08635-85-C-0054										
		10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. 62601F PROJECT NO. 1900 TASK NO. 70 WORK UNIT ACCESSION NO. 29										
11. TITLE (Include Security Classification) Evaluation and Prediction of Henry's Law Constants and Aqueous Solubilities for Solvents and Hydrocarbon Fuel Components												
12. PERSONAL AUTHOR(S) Howe, G.B.; Mullins, M.E.; Rogers, T.N.												
13a. TYPE OF REPORT Final	13b. TIME COVERED FROM Feb 85 TO Sep 86	14. DATE OF REPORT (Year, Month, Day) September 1987	15. PAGE COUNT 378									
16. SUPPLEMENTARY NOTATION Availability of this report is specified on reverse of front cover.												
17. COSATI CODES <table border="1"><tr><th>FIELD</th><th>GROUP</th><th>SUB-GROUP</th></tr><tr><td>07</td><td>01</td><td></td></tr><tr><td>07</td><td>04</td><td></td></tr></table>		FIELD	GROUP	SUB-GROUP	07	01		07	04		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number) Volatile organics, solvents, fuels, Henry's law constants, aqueous solubilities, air-water distribution.	
FIELD	GROUP	SUB-GROUP										
07	01											
07	04											
19. ABSTRACT (Continue on reverse if necessary and identify by block number) Laboratory measurements of Henry's law constants are reported for 51 chemicals spanning a wide range of chemical structures and volatilities. A static headspace method (Equilibrium Partitioning in Closed Systems, referred to as EPICS) was used to measure Henry's Law Constant, with the standard batch air-stripping method used as a check. An average precision of 5 percent was obtained for the EPICS runs, and the Henry's law constants agreed reasonably well (within 10 percent) with the batch air-stripping results and other reported experimental values. Measurements were conducted over a temperature range of 10-30°C, and the data were correlated with a temperature regression equation coupled with a temperature-dependent error term based on 95 percent confidence limits. The aqueous solubilities of the study compounds were also determined via the shake-flask method at temperatures of 10, 20, and 30 degrees Celsius. Finally, the results of this study were incorporated into a thermodynamic correlation (UNIFAC), based on chemical structure, which allows the prediction of Henry's law constants and aqueous solubilities for a wide variety of pure compounds and mixtures. (Cont'd)												
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT <input type="checkbox"/> UNCLASSIFIED/UNLIMITED <input type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS		21. ABSTRACT SECURITY CLASSIFICATION										
22a. NAME OF RESPONSIBLE INDIVIDUAL		22b. TELEPHONE (Include Area Code)	22c. OFFICE SYMBOL									

ITEM 19. ABSTRACT (Cont'd)

in dilute aqueous solutions. Volume II: Experimental Henry's Law Data (Volume II of III)

This report is presented in three volumes. Volume I contains the technical discussion and tabulated values of Henry's law constants and aqueous solubilities. Volume II contains the experimental Henry's law data. Volume III contains the experimental solubility data and the Fortran source code for the simplex UNIFAC parameter fitting and the interactive program for calculating Henry's law constants and aqueous solubilities.

22-0-7-Vii



Accession For	
NTIS CRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By _____	
Distribution/	
Availability Codes	
Distr	Final and/or Special
A-1	-

EXECUTIVE SUMMARY

The Installation Restoration program (IRP) underway at numerous Air Force bases has identified several sites with contaminated soil and groundwater. This subsurface contamination is the result of fuels, cleaning solvents, and degreasers entering the subsurface environment from accidental spills, leaking storage tanks, and past disposal practices. HQ AFESC/RDVW is conducting research aimed at developing treatment strategies for groundwater cleanup, and studying the fate and transport of contaminants in subsurface systems. Many of the contaminants of concern are volatile by nature, and a knowledge of their air-water distribution and aqueous solubility is needed to assess the compounds treatability and to support the basic laboratory studies.

The objectives of this research were to develop Henry's law constants and aqueous solubilities as a function of temperature, for a variety of organic compounds of Air Force concern (Table 1). Secondary objectives were to determine what effect mixed organics, in an aqueous solution, exhibit on individual Henry's law constants and evaluate various methods used to predict Henry's law constants.

This report documents experimentally determined values of Henry's law constants and aqueous solubility for 51 compounds of Air Force concern. The report is presented in three volumes. Volume I contains the technical discussion and tabulated values of Henry's law constants and aqueous solubilities. Volume II and III contain all the raw data and the fortran source code for an interactive program used to predict the chemical parameters.

Many of the contaminants of concern are volatile by nature, and a knowledge of their air-water distribution is required for the design of treatment processes and for providing insight into their environmental fate and transport. A static headspace method (Equilibrium Partitioning In Closed Systems, referred to as EPICS) was used to measure the Henry's law constants, with the standard batch air stripping method used as a check.

The Henry's constants were determined as a function of tempertaure from 10 to 30 °C (Table 11) and these values were then used to generate temperature regression equations (Table 8). Generally speaking the EPICS' results from this study agree well with other published results (Table 12). However, for many of the compounds reported here, confirmed values of Henry's constant do not exist in the literature, and if they do, values are rarely reported as a function of temperature with rigorous statistics.

Solubility data for organic compounds in water are important for environmental studies because they provide fundamental information necessary to predict transport in aqueous systems. This data may also be used to predict carbon sorption of contaminants, and the air-or steam-stripping behavior for a given compound. The aqueous solubility of the 51 study

compounds were determined at 10, 20, and 30°C (Table 14). Three different methods were used, but the majority of the data were collected using a shake-flask technique. Although the solubilities were not a strong function of temperature over the range studied (i.e., 10-30 °C), several general trends were noted. First, the solubility of the halogenated hydrocarbons increased with temperature. Second, the solubility of the substituted aromatic hydrocarbons increased with temperature. Finally, maxima and minima are observed for a wide range of compounds without any general trend that can be demonstrated to be statistically significant.

Groundwater contamination is often characterized by the presence of several different contaminants rather than one single compound. For this reason, studies were conducted to determine whether the presence of other compounds would affect the Henry's law constant of a single compound. Deviations from ideal behavior were observed (pg 52), but confirming experiments were not performed. Although the results were not conclusive, the project team believes the observed interactions were real and reproducible.

It would not be feasible to experimentally determine Henry's law constants for all chemical compounds. There will be times when a Henry's law constant is needed but an experimentally determined value is not reported and the situation does not permit a laboratory study to determine the constant. For this reason, a technique to accurately estimate Henry's constant using a minimum of physiochemical properties would be useful. Three different thermodynamic techniques for correlating experimental Henry's law constants were examined (page 61). The techniques were examined to determine their applicability to environmental systems and their predictive capacity for unmeasured multicomponent systems. The UNIFAC method proved to be the most effective way of utilizing the data base developed during this project. A computer algorithm to fit the current data to a new environmental UNIFAC binary interaction data base was developed and a portion of the experimental data collected was incorporated into this new data base. The new data base creates improvement in the predictions generated by UNIFAC in the dilute concentration regime (Figures 13 through 16).

PREFACE

This report was prepared by the Research Triangle Institute, Research Triangle Park NC 27707, under Contract No. F08635-85-C-0054. The AFESC/RDVW Project Officer was Captain Richard A. Ashworth.

The report documents Henry's law constants and aqueous solubilities, as a function of temperature, for 51 compounds of Air Force concern. The study was performed between February 1985 and September 1986.

This report is presented in three volumes. Volume I contains the technical discussion and the tabulated values of Henry's law constants and aqueous solubilities. Volume II contains the experimental Henry's law data. Volume III contains the experimental solubility data and the Fortran source code for the simplex UNIFAC parameter fitting and the interactive program for calculating Henry's law constants and aqueous solubilities.

Mention of trademarks and trade names of material and equipment does not constitute endorsement or recommendation for use by the Air Force, nor can the report be used for advertising the product.

This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

Richard A. Ashworth

RICHARD A. ASHWORTH, Capt, USAF, BSC
Project Officer

Lawrence D. Hokanson

LAWRENCE D. HOKANSON, Lt Col, USAF
Director, Engineering and Services
Laboratory

Thomas J. Walker

THOMAS J. WALKER, Lt Col, USAF, BSC
Chief, Environics Division

TABLE OF CONTENTS

Title	Page
APPENDIX A - Summary of Literature Search.....	1
APPENDIX B Summary of EPICS Results.....	19

Section
C or D

are included in this volume. KeyWords:
Water pollution Soil contamination

APPENDIX A
SUMMARY OF LITERATURE SEARCH

This is a self-contained document with its own internal style which, varies from our format.

SUMMARY OF LITERATURE SEARCH FINDINGS

The literature search initiated for this project may be divided into three main areas: (1) methodologies for measuring or estimating Henry's Law constants; (2) techniques for determining aqueous solubilities of volatile organics; and (3) group contribution correlations for VLE prediction. A thorough computer keyword search was supplemented by a manual investigation of the literature. Data bases used in the computer phase of the search include NTIS, COMPENDEX, CHEMICAL ABSTRACTS, WATERNET, POLLUTION ABSTRACTS, ENVIROLINE, and BIOSIS PREVIEWS.

A number of articles were found concerning Henry's Law constants for volatile organic compounds. The major measurement techniques discussed in the literature to date are inert gas stripping (batch air stripping in a bubble-purge column) and headspace methods such as EPICS. Procedures also exist for estimating Henry's Law constant from theoretical considerations and/or component physical property data, with particularly widespread use currently being made of crude, often highly suspect values calculated from the ratio of the organic's vapor pressure to its aqueous solubility limit. Finally, articles were found covering headspace analysis of trace organics, headspace concentration methods such as the purge-and-trap technique, and continuous organic extraction of aqueous samples. The latter two subjects are of importance to this project since they can be used to overcome detection limit problems and allow GC injection of non-aqueous liquid samples, respectively. Experimental Henry's constant and solubility data obtained during this study

will be compared to values given in the comprehensive listing of Mackay and Shiu (1981).

Methodologies for aqueous solubility measurement found in the literature fall into three categories: High Performance Liquid Chromatography (HPLC) generator column analysis, nephelometry (turbidity measurements), and the "shake-flask" technique which involves GC headspace analysis or UV liquid-phase detection. Shake-flask analysis, according to various authors, is accurate but time-consuming (several hours of liquid sample equilibration time are required), while the HPLC method, with a large bead surface area for organic-water contact, has a run time of only a few minutes. In this project, nephelometry will be used to check the experimental solubilities for selected chemicals arrived at by the shake-flask and HPLC methods.

The final major grouping of articles from the literature search centers around group contribution (chemical structure) correlations for trace organic physical properties. Procedures exist at present for calculating such quantities as activity coefficients in multicomponent aqueous solutions, pure component organic saturation pressures, and octanol-water partition coefficients. The type of correlation envisioned for this project would be similar in form and usage to the UNIFAC (UNIquac Functional-group Activity Coefficient) activity coefficient model described by Fredenslund, et al. (1975). Isolation of the individual functional group influences on partitioning behavior for various homologous series will be accomplished using the method for octanol-water partition coefficients given in the definitive paper by Leo, et al. (1971). If necessary, other correlation forms found in the literature, such as a nomograph or a correlation of Henry's constant against known physical properties, will be tried in an effort to satisfy Air Force prediction requirements.

The following literature listing summarizes the articles collected to date from the combined computer and manual literature search. Additional articles of interest to the Air Force have been ordered, and the list will be updated as they are received.

I. Determination of Henry's Law Constant

- Chian, E. S. K., and P. P. K. Kuo. 1977. Distillation/Headspace/Gas Chromatographic Analysis for Volatile Polar Organics at ppb Level. Environ. Sci. Tech. 11(3):282-285.
- Cotterman, R. L., and J. M. Prausnitz. 1985. Flash Calculations for Continuous or Semicontinuous Mixtures Using an Equation of State. Ind. Engr. Chem. Proc. Des. Dev. 24:434-443.
- Cowen, W. F., and R. K. Baynes. 1980. Estimated Application of Gas Chromatographic Headspace Analysis to Priority Pollutants. J. Environ. Sci. Health. A15(5):413-427.
- Dietz, E. A., Jr., and K. F. Singley. 1979. Determination of Chlorinated Hydrocarbons in Water by Headspace Gas Chromatography. Anal. Chem. 51(11):1809-1814.
- Dilling, W. L. 1977. Interphase Transfer Processes. II. Evaporation Rates of Chloro Methanes, Ethanes, Ethylenes, Propanes, and Propylenes from Dilute Aqueous Solutions: Comparisons with Theoretical Predictions. Environ. Sci. Tech. 11(4):405-409.
- Dilling, W. L., N. B. Tefetiller, and G. J. Kallos. 1975. Evaporation Rates and Reactivities of Methylene Chloride, Chloroform, 1,1,1-Trichloroethane, Trichloroethylene, Tetrachloroethylene, and Other Chlorinated in Dilute Aqueous Solutions. Environ. Sci. Tech. 9(9):833-838.
- Fredenslund, A., R. L. Jones, and J. M. Prausnitz. 1975. Group-Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures. AICHE J. 21(6):1086-1099.
- Gossett, J. M., and A. H. Lincoff. 1981. Solute-Gas Equilibria in Multi-Organic Aqueous Systems. Final Report. Air Force Office of Scientific Research, Grant No. AFOSR-81-0074. 33 pp.
- Grobe, R. L. 1980. Introduction. J. Environ. Sci. Health. A15(5):379-391.
- Grote, J. O., and R. G. Westendorf. An Automatic Purge and Trap Concentrator. 1979. Am. Lab. pp. 61-65.
- Hunter-Smith, R. J., P. W. Balls, and P. S. Liss. 1983. Henry's Law Constants and the Air-Sea Exchange of Various Low Molecular Weight Halocarbon Gases. Tellus. 35B:170-176.
- Hwang, S. T. 1982. Toxic Emissions from Land-Disposal Facilities. Environ. Prog. 1(11):46-52.

- Ioff, B. V., and A. J. Vitenberg. 1984. Headspace Analysis and Related Methods in Gas Chromatography. New York: John Wiley & Sons.
- Leighton, D. T., and J. M. Calo. 1981. Distribution Coefficients of Chlorinated Hydrocarbons in Dilute Air-Water Systems for Groundwater Contamination Applications. *J. Chem. Engr. Data* 26:382-385.
- Leo, A., C. Hansch, and D. Elkins. 1971. Partition Coefficients and their Uses. *Chem. Rev.* 71(6):525-554.
- Leroi, J., et al. 1977. Accurate Measurement of Activity Coefficients at Infinite Dilution by Inert Gas Stripping and Gas Chromatography. *Ind. Engr. Chem. Proc. Des. Dev.* 16(1):139-144.
- Lichtenbelt, J. H., and B. J. Schram. 1985. Vapor-Liquid Equilibrium of Water-Acetone-Air at Ambient Temperatures and Pressures. An Analysis of Different VLE-Fitting Methods. *Ind. Engr. Chem. Proc. Des. Dev.* 24:391-397.
- Lincoff, A. H., and J. M. Gossett. 1984. The Determination of Henry's Constant for Volatile Organics by Equilibrium Partitioning in Closed Systems. In: *Gas Transfer at Water Surfaces*. pp. 17-25.
- Liss, P. S., and P. G. Slater. 1974. Flux of Gases Across the Air-Sea Interface. *Nature*. 247:181-184.
- Mabey, W. R., J. H. Smith, R. T. Podoll, et al. 1982. Aquatic Fate Process Data for Organic Priority Pollutants. Section 4: Calculation of Partition Coefficients of Organic Chemicals in Aquatic Environments. Final Report. Environmental Protection Agency. EPA Report No. 440/4-81-014. December.
- Mackay, D., and P. J. Leinonen. 1975. Rate of Evaporation of Low-Solubility Contaminants from Water Bodies to Atmosphere. *Environ. Sci. Tech.* 9(13): 1178-1180.
- Mackay, D., and W. Y. Shiu. 1981. Critical Review of Henry's Law Constants for Chemicals of Environmental Interest. *J. Phys. Chem. Ref. Data* 10(4): 1175-1199.
- Mackay, D., W. Y. Shiu, and R. P. Sutherland. 1979. Determination of Air-Water Henry's Law Constants for Hydrophobic Pollutants. *Environ. Sci. Tech.* 13(3):333-337.
- McAullife, C. 1971. GC Determination of Solutes by Multiple Phase Equilibration. *Chem. Tech.* 1.
- McCarty, P. L. 1980. Organics in Water--An Engineering Challenge. *J. Environ. Engr. Div.* pp. 1-17.
- McConnell, G., D. M. Ferguson, and C. R. Pearson. 1975. Chlorinated Hydrocarbons and the Environment. *Endeavour*. 34.

- McNally, M. E., and R. L. Grob. 1985. A Review: Current Applications of Static and Dynamic Headspace Analysis. Part One: Environmental Applications. Am. Lab. pp. 20-33.
- Mesnage, J., and A. A. Marsan. 1971. Vapor-Liquid Equilibrium at Atmospheric Pressure. J. Chem. Engr. Data. 16(4):434-439.
- Monfort, J. P., and J. L. Perez. 1978. Henry's Constants of Normal Mixtures Calculated with a Modified Pierotti Theory Using Temperature-Dependent Hard Core Diameters. Chem. Engr. J. 16:205-209.
- Mousa, A. H. N. 1984. Prediction of Henry's Constant by Gas Chromatography. J. Chem. Engr. Jpn. 17(2):206-208.
- Ng, S., H. G. Harris, and J. M. Prausnitz. 1969. Henry's Constants for Methane, Ethane, Ethylene, Propane, and Propylene in Octadecane, Eicosane, and Docosane. J. Chem. Engr. Data 14(4):482-483.
- Nicholson, B. C., B. P. Maguire, and D. B. Bursill. 1984. Henry's Law Constants for the Trihalomethanes: Effects of Water Composition and Temperature. Environ. Sci. Tech. 18:518-521.
- Osinga, M. 1979. Rigidity, Lipophilicity, and Henry's Constant. Letter to Am. Chem. Soc. J. 101(6):1621-1622.
- Richon, D., and H. Renon. 1980. Infinite Dilution Henry's Constants of Light Hydrocarbons in n-Hexadecane, n-Octadecane, and 2,2,4,4,6,8,8-Heptamethyl-nonane by Inert Gas Stripping. J. Chem. Engr. 25:59-80.
- Shaw, D. A., and T. F. Anderson. 1983. Use of Gas Chromatographic Headspace Analysis in Vapor-Liquid Equilibrium Data Collection. Ind. Engr. Chem. Fundam. 22:79-83.
- Singleton, J. A., and H. E. Pattee. 1980. A Preconcentration and Subsequent Gas Liquid Chromatographic Analysis Method for Trace Volatiles. JAOCs. December 1980. pp. 405-408.
- Southworth, G. R. 1982. Evaporation of Phenols from Synthetic Liquid Fuel Spills. Environ. Intl. 7:203-206.
- Spencer, W. F., and M. M. Cliath. 1968. Vapor Density of Dieldrin. Environ. Sci. Tech. 3(7):670-674.
- Stein, V. B., and R. S. Narang. 1981. Determination of Vinyl Chloride by Headspace Analysis by Photoionization Detection. Bull. Environ. Contam. Toxicol. 27:582-587.
- Symposium on Gas Chromatography. 1955. Report of Joint Meeting of Physical Methods Group, Microchemistry Group and Scottish Section on May 20, 1955. Analyst. 81:52-58.
- Umbreit, G. R. 1979. Chromatographic Anomalies. 1979. Chem. Tech. 7(2):101-106.

Umbreit, G. R., and R. L. Grob. 1980. Experimental Application of Gas Chromatographic Headspace Analysis to Priority Pollutants. *J. Environ. Sci. Health.* A15(5):429-466.

Van Ness, H. C., S. M. Byer, and R. E. Gibbs. 1973. Vapor-Liquid Equilibrium: An Appraisal of Data Reduction Methods. *AICHE J.* 19(2):238-244.

Wilson, A., and E. L. Simons. 1952. Vapor-Liquid Equilibria. 2-Propanol-Water System. *Ind. Eng. Chem.* 44:2214-2219.

Yoshizumi, K., K. Aoki, and I. Nouchi. 1984. Measurements of the Concentration in Rainwater and of the Henry's Law Constant of Hydrogen Peroxide. *Atmos. Environ.* 18(2):395-401.

II. Aqueous Solubility Measurement

- Ballinger, D., et al. 1981. A Method for the Determination of Sulphides in Water, Sewage and Effluents. *Wat. Pollut. Control.* pp. 648-654.
- Battino, R., and H. L. Clever. 1966. The Solubility of Gases in Liquids. *Chem. Rev.* 66:395.
- Benson, B. B., D. Krause, Jr., and M. A. Peterson. 1979. The Solubility and Isotopic Fractionation of Gases in Dilute Aqueous Solution. I. Oxygen. *J. Sol. Chem.* 8(9):655-690.
- Black, C., G. G. Joris, and H. S. Taylor. 1948. The Solubility of Water in Hydrocarbons. *J. Chem. Phys.* 16(5):537-543.
- Block, R. M., J. Dragun, and T. W. Kalonowski. 1984. Groundwater Contamination. Part 2: Health and Environmental Aspects of Setting Cleanup Criteria. *Chem. Engr.* November 26, 1984. pp. 70-72.
- Brass, H. J. 1980. The Analysis of Trihalomethanes in Drinking Water by Purge and Trap and Liquid-Liquid Extraction. *Am. Lab.* 12(7):23-30.
- Chameides, W. L., and D. D. Davis. 1983. Aqueous-Phase Source of Formic Acid in Clouds. *Nature.* 304(4):427-429.
- Cramer, S. D. 1984. Oxygen Solubility in Brines. *Ind. Engr. Chem. Proc. Des. Dev.* 23:618-620.
- Cramer, S. D. 1984. Solubility of Methane in Brines from 0 to 300°C. *Ind. Engr. Chem. Proc. Des. Dev.* 23:533-538.
- Cudor, P. M., and J. M. Prausnitz. 1972. Solubilities of Gases in Liquids at Elevated Temperatures. Henry's Constants for Hydrogen, Methane, and Ethane in Hexadecane, Bicyclohexyl, and Diphenylmethane. *J. Phys. Chem.* 76(4):598-601.
- Deland, M. R. 1980. Groundwater: A National Strategy. *Environ. Sci. Tech.* 14(5):517.
- Dragun, J., A. C. Kuffner, and R. W. Schneiter. 1984. Groundwater Contamination. Part 1: Transport and Transformations of Organic Chemicals. *Chem. Engr.* November 26, 1984. pp. 65-69.
- Everett, D. H., and C. T. H. Stoddart. 1961. *Trans. Faraday Soc.* 57:746-754.
- Federal Register. 1979. 44(53):16250-16278. March 16, 1979.

- Fernandez-Prini, R., and R. Crovett. 1985. A Critical Evaluation of the Solubility of Simple Inorganic Gases in Water at High Temperature. *AICHE J.* 31(3):513-516.
- Franks, F. 1966. Solute-Water Interactions and the Solubility Behaviour of Long-chain Paraffin Hydrocarbons. *Nature*. 210:87-88.
- Goodman, C. 1984. Predicting Mass Transfer Coefficients for Packed Tower Air Stripping of Dilute Organics. Thesis.
- Gross, R. L., Capt., and S. G. TerMaath, Maj. 1984. Packed Tower Aeration Strips Trichloroethylene from Groundwater. Submitted for Presentation at the 1984 Summer National Meeting of the American Institute of Chemical Engineers.
- Hollifield, H. C. 1979. Rapid Nephelometric Estimate of Water Solubility of Highly Insoluble Organic Chemicals of Environmental Interest. *Bull. Environ. Contam. Toxicol.* 23:579-586.
- Isacoff, E. G., and J. A. Bittner. 1979. Resin Adsorbent Takes on Chlororganics from Well Water. *Water & Sewage Works*. August 1979. pp. 41-42.
- Kabadi, V. N., and R. P. Danner. 1979. Nomograph Solves for Solubilities of Hydrocarbons in Water. *Hydrocarbon Proc.* 58(5):245-246.
- Karickhoff, S. W., and D. S. Brown. 1979. Determination of Octanol/Water Distribution Coefficients, Water Solubilities, and Sediment/Water Partition Coefficients for Hydrophobic Organic Pollutants. Final Report. Environmental Protection Agency. Report No. 600/4-79-032. 16 pp.
- Kavanaugh, M. C., and R. R. Trussell. 1980. Design of Aeration Towers to Strip Volatile Contaminants from Drinking Water. *J. Am. Water Works Assoc.* 72:684-692.
- Knepper, J. C., and J. W. Gorman. 1980. Statistical Analysis of Constrained Data Sets. *AICHE J.* 26(2):260-264.
- Mackay, D., R. Mascarenhas, and W. Y. Shiu. 1980. Aqueous Solubility of Polychlorinated Biphenyls. *Chemosphere*. 9:257-264.
- Mackay, D., and W. Y. Shiu. 1975. The Determination of the Solubility of Hydrocarbons in Aqueous Sodium Chloride Solutions. *Can. J. Chem. Engr.* 53:239-242.
- Mackay, D., and W. Y. Shiu. 1977. Aqueous Solubility of Polynuclear Aromatic Hydrocarbons. *J. Chem. Engr. Data* 22(4):399-402.
- May, W. E., et al. 1978. Development of an Aqueous Polynuclear Aromatic Hydrocarbon Standard Reference Material. National Bureau of Standards Special Publication 519. *Trace Organic Analysis: A New Frontier in Analytical Chemistry*. Proceedings of the 9th Material Research Symposium, April 10-13, 1978 at NBS Gaithersburg, Maryland.

- May, W. E., S. P. Wasik, and D. H. Freeman. 1978. Determination of the Solubility Behavior of Some Polycyclic Aromatic Hydrocarbons in Water. *Anal. Chem.* 50(7):997-1000.
- McAuliffe, C. 1966. Solubility in Water of Paraffin, Cycloparaffin, Olefin, Acetylene, Cycloolefin, and Aromatic Hydrocarbons. *J. Phys. Chem.* 70(4): 1267-1275.
- McCann, D. W., and R. P. Danner. 1984. Prediction of Second Virial Coefficients of Organic Compounds by a Group Contribution Method. *Ind. Engr. Chem. Proc. Des. Dev.* 23:529-533.
- McNally, M. E., and R. L. Grob. 1983. Determination of the Solubility Limits of Organic Priority Pollutants by Gas Chromatographic Headspace Analysis. *J. Chrom.* 260:23-32.
- Miller, R. E. 1984. Confidence Intervals and Hypothesis Tests. *Chem. Engr.* November 26, 1984. pp. 89-93.
- Nelson, T. P., J. R. Blacksmith, and J. L. Randall. 1985. Field Evaluation of Volatile Organic Compound Removal Efficiency for Full Scale Carbon Adsorption Systems. *Environ. Prog.* 4(1):14-19.
- Pearson, C. R., and G. McConnell. 1975. Chlorinated C₁ and C₂ Hydrocarbons in the Marine Environment. *Proc. R. Soc. Lond. B* 189:305-332.
- Peters. 1982. Comparison of Continuous Extractors for the Extraction and Concentration of Trace Organics from Water. *Anal. Chem.* 54:1913-1914.
- Petty, R. L. 1981. Determination of Benzene at Low Parts per Trillion Levels in Seawater. *Marine Chem.* 10:409-416.
- Plackett, R. L., and J. P. Burman. 1985. The Design of Optimum Multifactorial Experiments. Prepared for Information Services Center, Charleston Research. West Virginia Pulp & Paper Company. Charleston, South Carolina. 20 pp.
- Price, F. R., and C. Ponnamperuma. 1980. Analysis of Volatile Amines by GC. *Am. Lab.* 12(10):45-51.
- Rasmussen, R. A., S. D. Hoyt, and M. A. K. Khalil. 1982. Atmospheric Carbonyl Sulfide (OCS): Techniques for Measurement in Air and Water. *Chemosphere.* 11(9):869-875.
- Roberts, P. V., et al. 1985. Evaluating Two-Resistance Models for Air Stripping of Volatile Organic Contaminants in a Countercurrent Packed Column. *Environ. Sci. Tech.* 19:164-173.
- Safeguards for Groundwater. 1980. *Environ. Sci. Tech.* 14(1):38-44.

- Sanemasa, I., et al. 1981. Solubilities of Benzene and the Alkylbenzenes in Water--Method for Obtaining Aqueous Solutions Saturated with Vapors in Equilibrium with Organic Liquids. Chem. Ltrs. Chem. Soc. of Japan. pp. 225-228.
- Schneiter, R. W., J. Dragun, and T. G. Erler, III. 1984. Groundwater Contamination. Part 3: Remedial Action. Chem. Engr. November 26, 1984. pp. 73-78.
- Schwarz, F. P. 1980. Measurement of the Solubilities of Slightly Soluble Organic Liquids in Water by Elution Chromatography. Anal. Chem. 52:10-15.
- Silverman, N., and D. Tasslos. 1984. Prediction of Multicomponent Vapor-Liquid Equilibrium with the Wilson Equation: Effect of the Minimization Function and of the Quality of Binary Data. Ind. Engr. Chem. Proc. Des. Dev. 23:586-589.
- Stallings, R. L., T. N. Rogers, and M. E. Mullins. 1985. Air Stripping of Volatile Organics. Proceedings of Institute of Environmental Sciences. 5 pp.
- Statistical Distributions for Parameters of Environmental Concern. 1984. Draft Report. Prepared by RTI for Environmental Protection Agency. Contract No. 68-03-3149. Work Assignment 51-2.
- Stolzenburg, T. R., and A. W. Andren. 1983. Determination of the Aqueous Solubility of 4-Chlorobiphenyl. Anal. Chim. Acta 151:271-274.
- Swann, R. L., et al. 1983. A Rapid Method for the Estimation of the Environmental Parameters Octanol/Water Partition Coefficient, Soil Sorption Constant, Water to Air Ratio, and Water Solubility. Residue Reviews. 85:17-35.
- Tewari, Y. B., et al. 1982. Aqueous Solubilities and Octanol/Water Partition Coefficients of Binary Liquid Mixtures of Organic Compounds at 25°C. J. Sol. Chem. 11(6):435-445.
- Tewari, Y. B., et al. 1982. Aqueous Solubility and Octanol/Water Partition Coefficient of Organic Compounds at 25.0°C. J. Chem. Engr. Data 27:451-454.
- U.S. Environmental Protection Agency. 1982. Environmental Monitoring and Support Laboratory, Cincinnati, Ohio. Test Method. Purgeable Halocarbons--Method 601.
- Wasik, S. P., et al. Determination of the Vapor Pressure, Aqueous Solubility, and Octanol/Water Partition Coefficient of Hydrophobic Substances by Coupled Generator Column/Liquid Chromatographic Methods. Residue Rev. 85:29-41.

- Wauchope, R. D., and F. W. Getzen. 1972. Temperature Dependence of Solubilities in Water and Heats of Fusion of Solid Aromatic Hydrocarbons. *J. Chem. Engr. Data* 17(1):38-41.
- Westendorf, R. G. 1981. Development and Application of a Semiautomatic Purge and Trap Concentrator. *Am. Lab.* 13(10):88-95.
- Wilhelm, E., and R. Battino. 1973. Thermodynamic Functions of the Solubilities of Gases in Liquids at 25°C. *Chem. Rev.* 73(1):1-9.
- Wong, J. M., and K. P. Johnson. 1984. Thermodynamic Models for Nonrandom and Strongly Nonideal Liquid Mixtures. *Ind. Engr. Chem. Fundam.* 23:320-326.
- Yalkowsky, S. H., and S. C. Valvani. 1980. Solubility and Partitioning I: Solubility of Nonelectrolytes in Water. *J. Pharm. Sci.* 69(8):912-922.
- Zerpa, C. O., et al. 1979. Solubility of Cyclopropane in Aqueous Solutions of Potassium Chloride. *J. Chem. Engr. Data* 24(1):26-28.
- Zsolnay, A. 1974. Determination of Aromatic and Total Hydrocarbon Content in Submicrogram and Microgram Quantities in Aqueous Systems by Means of High Performance Liquid Chromatography. NBS Special Publication 409. Marine Pollution Monitoring (Petroleum). Proceedings of a Symposium and Workshop at NBS, Gaithersburg, Maryland, May 13-17, 1974.

III. Thermodynamic VLE Correlations

Abrams, D. S., Rec. Trav. Chim., Pays-Bas 69, 163, 1975.

Abrams, D. S., and J. M. Parusnitz, "Statistical Thermodynamics of Liquid Mixtures: A New Expression for the Excess Gibbs Energy of Partly or Completely Miscible Systems," AIChE Journal, Vol. 21:116, 1975.

Antunes, Carlos and Dimitrios Tassios, "Modified UNIFAC Model for the Prediction of Henry's Constants," New Jersey Institute of Technology, Newark, NJ.

Aranow, R. H., and L. Witten, "The Environmental Influence on the Behavior of Long Chain Molecules," J. Phys. Chem., Vol. 64:1643-1648, 1960.

Arbuckle, W. E., "Estimating Activity Coefficients for use in Calculating Environmental Parameters," Environ. Sci. Tech., Vol. 17:537-542, 1983.

Ball, F. X., W. Furst and H. Renon, "An NRTL Model for Representation and Prediction of Deviation from Ideality in Electrolyte Solutions Compared to the Models of Chen (1982) and Pitzer (1973)," AIChE J., Vol. 31(3):392-399, 1985.

Bastos, J. C., M. E. Soares and A. G. Medina, "Selection of Solvents for Extractive Distillation. A Data Bank for Activity Coefficients at Infinite Dilution," Ind. Engr. Chem. Proc. Des. Dev., Vol. 24(2):420-426, 1985.

Black, C., G. Joris and H. Taylor, "The Solubility of Water in Hydrocarbons," Journal of Chem. Phys., Vol. 16:537, 1948.

Bondi, "A Physical Properties of Molecular Crystals, Liquids, and Gasses," Academic Press, 1968.

Burkhard, L. P., "Estimation of Vapor Pressure for Halogenated Aromatic Hydrocarbon by a Group-Contribution Method," Ind. Engr. Chem. Fundam., Vol. 24:119-120, 1985.

Burris, D. R. and W. G. MacIntyre, "Water Solubility Behavior of Binary Hydrocarbon Mixtures," Virginia Institute of Marine Sciences, School of Medicine, College of William and Mary, Gloucester, Virginia, 1984.

Burris, D. R. and W. G. MacIntyre, "A Thermodynamic Study of Solutions of Liquid Hydrocarbon Mixtures in Water," Virginia Institute of Marine Sciences, School of Medicine, College of William and Mary, Gloucester, Virginia, 1986.

Butler, J., C. Ramchandani and D. Thomson, "The Solubility of Non-Electrolytes: Part I. The Free Energy of Hydration of Some Aliphatic Alcohols," J. Chem. Soc., p. 952, 1935.

Chakravarty, T., C. W. White and W. D. Seider, "Computation of Phase Equilibrium: Optimization with Thermodynamic Inconsistency," AIChE J., Vol. 31(2):316-321, 1985.

Chimowitz, W. H., et al., "Local Models for Representing Phase Equilibria in Multicomponent Nonideal Vapor-Liquid and Liquid-Liquid Systems. 2. Application to Process Design," Ind. Engr. Chem. Proc. Des. Dev., Vol. 23:609-618, 1984.

Cruickshank, A. H. B., D. H. Everett and M. T. Westaway, 1965.

Deal, C. and E. L. Deer, "Selectivity and Solvency in Aromatics Recovery." Ind. Eng. Chem. Process Des. Dev., Vol. 3:394, 1964.

Derr, E. L. and C. H. Deal, "Analytical Solutions of Groups: Correlation of Activity Coefficients Through Structural Group Parameters," I. Chem. E. Symp. Ser., Vol. 32:337, 1969.

Derr, E. L. and C. H. Deal, "Predicted Composition During Mixed Solvent Evaporation from Resin Solutions Using the Analytical Solution of Group Method," Advan. Chem. Ser., Vol. 124:11, 1973.

Donahue, M. D. and J. M. Prausnitz, "Combinatorial Entropy of Mixing Molecules that Differ in Size and Shape. A Simple Approximation for Binary and Multicomponent Mixtures," University of California, Berkeley, CA, October 1974.

Donahue, M. D. and J. M. Prausnitz, Can J. Chem., Vol. 53:1586, 1975.

Donahue, J. and F. Bartell, "The Boundary Tension at Water-Organic Liquid Interfaces," J. Phys. Chem., Vol. 56:480, 1952.

Duhem, P. and J. Vidal, "Extension of the Dilutor Method to Measurement of High Activity Coefficients at Infinite Dilution," Fluid Phase Equil., Vol. 2:231-235, 1978.

Fredenslund, A., et al., "Computerized Design of Multicomponent Distillation Columns using the UNIFAC Group Contribution Method for Calculation of Activity Coefficients," Ing. Engr. Chem. Proc. Des. Dev., Vol. 16(4):450-462, 1977.

Fredenslund, A., J. Gmehling and P. Rasmussen, "Vapor-liquid Equilibria using UNIFAC," Elsevier, Amsterdam, 1977.

Fredenslund A., and P. Rasmussen, Fluid Phase Equil., Vol. 24: 115, 1985.

Fredenslund, A., R. L. Jones and J. M. Prausnitz, "Group-Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures," AICHE Journal, Vol. 21:1086-1099, 1975.

Flory, P. J., "Statistical Thermodynamics of Liquid Mixtures," J. Am. Chem. Soc., Vol. 87(9):1833, 1965.

Fujita, T., J. Iwasa and C. Hansch, J. Am. Chem. Soc., Vol. 86:5175, 1964.

Gmehling, J., "Group Contribution Methods for the Estimation Activity Coefficients," presented at the Fourth International Conference on Fluid Properties and Phase Equilibria, Helsingor, Denmark, May 1986, Fluid Phase Equilibria, to be published.

- Gmehling, J., P. Rasmussen and A. Fredenslund. "Vapor-Liquid Equilibria by UNIFAC Group Contribution." Revision and Extension II. Ind. Eng. Chem. Process Des. Dev., 1982.
- Goldstein, D. J., "Air and Stream Stripping of Toxic Pollutants." U.S. Environmental Protection Agency Report No. 68-03-002, Vol. II, 1982.
- Gossett, J. M., "Anaerobic Degradation of C₁ and C₂ Chlorinated Hydrocarbons." Final Report. Air Force Engineering and Services Center, Tyndall Air Force Base, Florida. ESL-TR-8538, 123-149.
- Hayden, J. G. and J. P. O'Connell. "A Generalized Method for Predicting Second Viral Coefficients." Ind. Engr. Chem. Proce. Des. Dev., Vol. 14(3):209-216, 1975.
- Hoshino, D., et al., "Prediction of Vapor Pressure for Substituted Benzenes by a Group-Contribution Method." Ind. Engr. Chem. Fund., Vol. 24:11-114, 1985.
- Hy, Y., E. Azevedo, D. Ludecke and J. Prausnitz. "Thermodynamics of Associated Solutions: Henry's Constants for Nonpolar Solutes in Water." Fluid Phase Equilibria, Vol. 17:303-321, 1984.
- Kikic, I. L., P. Alessi, P. Rasmussen and A. Frendenslund. "On the Combinatorial Part of the UNIFAC and UNIQUAC Models." Can. J. Chem. Eng., Vol. 58:253-258, 1980.
- Langmuir, I., "The Distribution and Orientation of Molecules." Third Colloid Symposium Monograph, Vol. 48, 1925.
- Leo, A., C. Hansch and D. Elkins. "Partition Coefficients and their Uses." Chem. Rev. 71:525-555, 1971.
- Lin, H., "Modified Soave Equation for State for Phase Equilibrium Calculations." Ind. Engr. Chem. Proce. Des. Dev., Vol. 19(3):501-505, 1980.
- Lo, T. C., H. Bieber and A. Karr. "Vapor-Liquid Equilibrium of n-Petane-Acetone." J. Chem. Eng. Data, Vol. 7:327, 1962.
- Mackay, D. (technical note). Environ. Sci. Technol., Vol. 11:1219, 1977.
- Münz, C. and P. V. Roberts. "Effects of Solute Concentration and Cosolvents of the Aqueous Activity Coefficient of Halogenated Hydrocarbons." Civing Engineering Department, Stanford University, Stanford, California.
- Nicolaides, G., "Optimal Measurement and Correlation of Binary Liquid Mixture Nonidealities." Ph.D. Thesis, Univ. of Illinois, 1977.
- Nicolaides, G. and C. Eckert. "Optimal Representation of Binary Liquid Mixture Nonidealities." Ind. Eng. Chem. Fundam., Vol. 17:331, 1978.
- Nothangel, K., D. S. Abrams and J. M. Prausnitz. "Generalized Correlation for Fugacity Coefficients in Mixtures at Moderate Pressures." Ind. Engr. Chem. Proc. Des. Dev., Vol. 12(1):25-35, 1973.

- Oyre, R. V. and J. M. Prausnitz, "Multicomponent Equilibria with the Wilson Equation," Ind. Eng. Chem., Vol. 57:19, 1965.
- Palmer, D. A., "Predicting Equilibrium Relations for Maverick Mixtures," Chem. Eng. (N.Y.), Vol. 82:12, 80, 1975.
- Patterson, D. and M. Barbe, "Enthalpy-Entropy Compensation and Order in Alkane and Aqueous Systems," J. Phys. Chem., Vol. 80(21):2435-2436, 1976.
- Pierotti, G., C. Deal and E. Derr, "Activity Coefficients and Molecular Structure," Ind. Eng. Chem., Vol. 51:95, 1959.
- Prausnitz, J. M., E. Azevedo and R. Lichtenthaler, "Molecular Thermodynamics of Fluid-Phase Equilibria," Second Edition, Prentice-Hall, 1986.
- Rasmussen, P. and A. Fredenslund, "Prediction of Separation Factors Using Group Contribution Methods a Review," Marcel Dekker, Inc., 1979.
- Rasmussen, P. and A. Fredenslund, "Separation and Purif," Methods 7:147, 1978.
- Renon, H. and J. M. Prausnitz, "Local Composition in Thermodynamic Excess Functions for Liquid Mixtures," AIChE J., Vol. 14:135, 1968.
- Reid, R. C., J. M. Prausnitz and T. K. Sherwood, "The Properties of Gases and Liquids," Third Edition, McGraw-Hill Book Co., New York, 1977.
- Schreiber, L. and C. Eckert, "Use of Infinite Dilution Activity Coefficients with the Wilson's Equation," Ind. Eng. Chem. Process Des. Dev., Vol. 10:572, 1971.
- Siedel, A., "Solubilities of Organic Compounds," D. Van Nostrand Co., New York, 1941.
- Skold-Jorgensen, S., et al., "Vapor-Liquid Equilibria by UNIFAC Group Contribution," Revision and Extension, Ind. Engr. Chem. Proce. Des. Dev., Vol. 18(4):714-722, 1979.
- Soave, G., "Equilibrium Constants from a Modified Redlich-Kwong Equation of State," J. Eng. Sci., Vol. 27:1197-1203, 1972.
- Staverman, A. J., "The Entropy of High Polymer Solutions. Generalization of Formulae," August 1949.
- Staverman, A. J., Rec. Trav. Chim., Pays-Bas 69:163, 1975.
- Tancrede, P., et al., "Interactions in Alkane Systems by Depolarized Rayleigh Scattering and Calorimetry," J. Chem. Soc. Faraday Trans., Vol. 73(2): 15-39, 1977.
- Tiegs, D., P. Rasmussen, J. Gmehling, A. Frendenslund, "Vapor-Liquid Equilibria by UNIFAC Group Contribution," Revision and Extension 3, Ind. Eng. Chem. Proc. Des. Dev., in press.

Tsonopoulos, C. and J. M. Prausnitz, "Activity Coefficients of Aromatic Solutes in Dilute Aqueous Solutions," Ind. Engr. Chem. Fundam., Vol. 10(4):593-600, 1971.

Warner, H., J. Cohen and J. Ireland, "Determination of Henry's Law Constants of Selected Priority Pollutants," Draft Report from Municipal Environmental Research Lab., Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, Ohio, 1980.

Wilson, G. M., "A New Expression for the Excess Free Energy of Mixing," J. Am. Chem. Soc., Vol. 86:127, 1964.

Wilson, G. M. and C. H. Deal, "Activity Coefficients and Molecular Structure," Ind. Engr. Chem. Fundam., Vol. 1(1):20-23, 1962.

APPENDIX B
SUMMARY OF EPICS RESULTS

SUMMARY OF EPICS RESULTS

Calculated statistical quantities in this Appendix include the coefficient of variation (relative standard deviation) for all replicate Henry's law constant observations; the temperature regression parameters (slope and y-intercept) and associated correlation coefficient for each component; and the Student's "T"-test confidence bands for both the raw data and the temperature regression predictions. Appropriate temperature regression and confidence interval plots have been generated to present the data graphically.

Divided according to component, the data analysis information for each chemical consists of the following:

- Two-page tabulation of the injection peak areas, Henry's law constant estimates, and Coefficient of Variation (COV) values for the component at five temperatures (10, 15, 20, 25 and 30°C)
- Temperature regression plot ($\ln H$ versus $1/T$)
- Plot showing the 95 percent confidence band on the temperature regression predictions
- Plot illustrating the 95 percent confidence limits (lower and upper) on the averages of the estimates calculated at each temperature.

All of this information is presented in this Appendix for 48 of the original 51 compounds of interest. Notice, however, that the temperature regression plot and associated confidence band plot for component 102 (n-hexane) have been omitted from this compilation. This is because the negligible temperature dependence of the raw data rendered the regression analysis meaningless.

A brief discussion of the phenol results is also warranted here because the measured Henry's law constants are significantly higher than other published data. This observation is explained by recalling that phenol self-associates strongly in aqueous solution even at low environmental concentrations. Equilibrium air-water partitioning of phenol therefore consists of competing equilibria: equilibrium between the phenol monomer and phenol "chains" in the liquid phase, and air-water distribution of the monomer. The EPICS technique measures the air-water partitioning of the monomer only; calculated ratios of vapor pressure to aqueous solubility are based instead on the bulk liquid-phase phenol concentration. In other words, calculated Henry's law constants for highly nonideal chemicals such as phenol will be much lower than experimental values because the overall solubility limit is typically much higher than the true monomer solution concentration. A good model of equilibrium partitioning behavior in such systems should include a realistic representation of the multiple equilibria involved.

Serial Dilution Results with Example Curves

COMPONENT ID INDEX AND SERIAL DILUTION RESULTS

Component ID Number	Component Name	Serial Dilution Correlation Coefficient (r^2)
101	n-nonane	0.998
2	n-hexane	0.998
102	n-hexane	
3	2-methylpentane	1.000
103	2-methylpentane	
4	cyclohexane	0.998
5	1,2-dichlorobenzene	1.000
105	1,2-dichlorobenzene	
6	chlorobenzene	0.999
7	1,3-dichlorobenzene	0.997
107	1,3-dichlorobenzene	
8	1,4-dichlorobenzene	0.997
108	1,4-dichlorobenzene	
9	o-xylene	0.998
10	p-xylene	0.998
11	m-xylene	0.997
12	propylbenzene	0.997
13	ethylbenzene	0.990
113	ethylbenzene	
14	toluene	1.000
15	benzene	0.982
16	phenol	0.864
17	methyl ethylbenzene	0.998
18	1,1-dichloroethane	1.000
19	1,2-dichloroethane	1.000
119	1,2-dichloroethane	0.9993
20	1,1,1-trichloroethane	0.999
21	1,1,2-trichloroethane	0.998
121	1,1,2-trichloroethane	
22	cis-dichloroethylene	0.996
23	trans-dichloroethylene	0.995
24	tetrachloroethylene	1.000
25	trichloroethylene	1.000
26	naphthalene	0.997
27	tetralin (1,2,3,4-tetrahydronaphthane)	0.996
127	tetralin	
28	decalin	0.989
128	decalin	
29	anthracene	-----
30	vinyl chloride	1.000
130	vinyl chloride	
31	chloroethane	0.999
32	hexachloroethane	0.992
132	hexachloroethane	

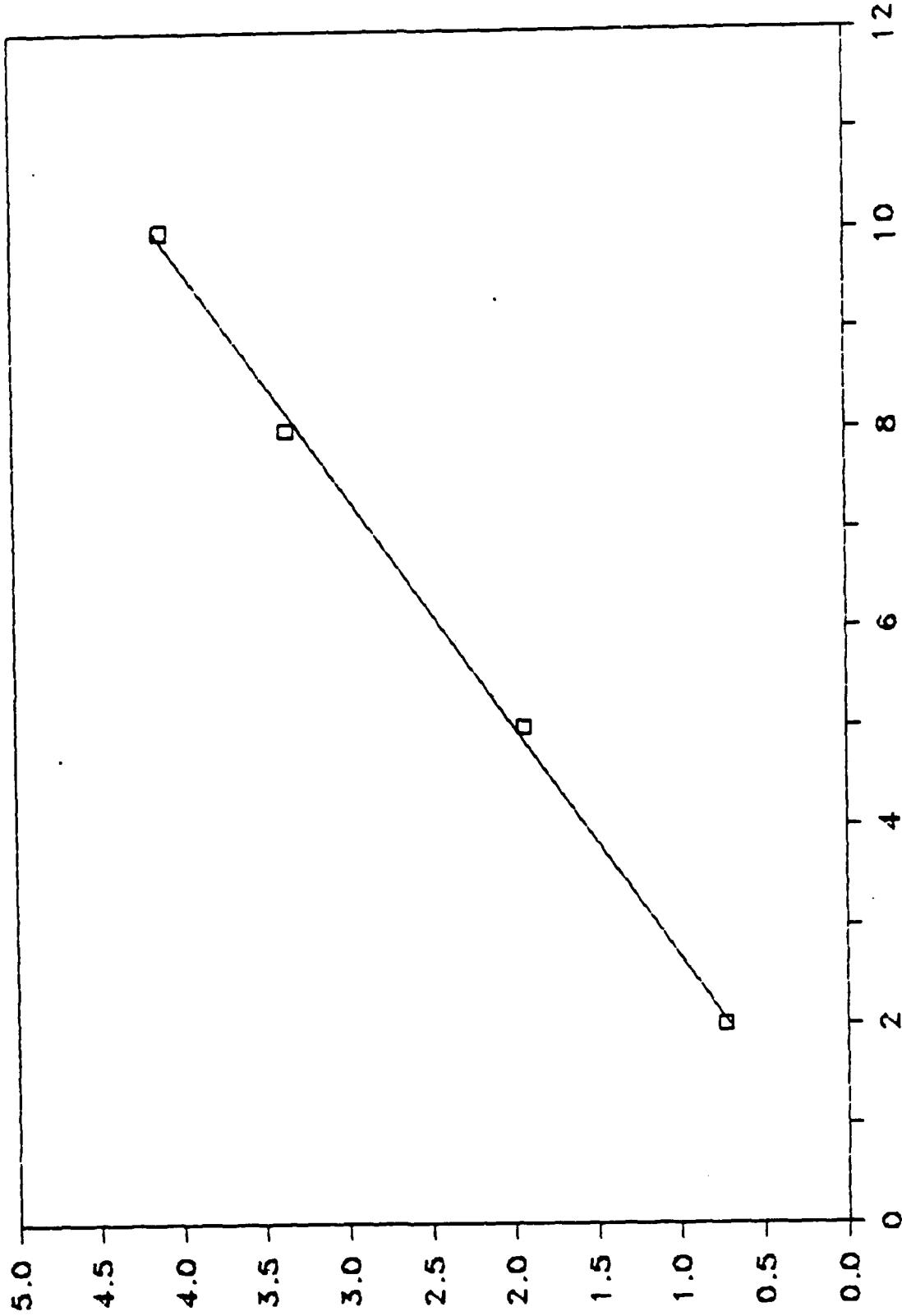
COMPONENT ID INDEX AND SERIAL DILUTION RESULTS

PAGE 2

Component ID Number	Component Name	Serial Dilution Correlation Coefficient (r^2)
33	carbon tetrachloride	0.999
34	1,3, 5-trimethylbenzene (mesitylene)	0.997
35	bis (2-ethylhexyl)phthalate (dioctyl phthalate)	-----
36	ethylene dibromide	1.000
136		0.9996
37	1, 1-dichloroethylene (vinylidene chloride)	0.996
38	methylene chloride	0.9993
50	methylene chloride	0.9997
39	chloroform	0.9998
49	chloroform	0.9932
43	1,1,2,2-tetrachloroethane	0.9921
44	1,2-dichloropropane	0.9999
45	dibromochloromethane	0.9990
46	1,2,4-trichlorobenzene	0.9989
47	2,4-dimethylphenol	0.9316
51	1,1,2-trichlorotrifluoroethane	0.9953
52	methyl ethyl ketone (MEK)	0.9970
152	methyl ethyl ketone (MEK)	
53	methyl isobutyl ketone (MIBK)	0.9878
153	methyl isobutyl ketone (MIBK)	-----
54	methyl cellosolve	-----
55	bis (2-chloroethyl) ether	-----
56	trichlorofluoromethane	-----

SERIAL DILUTION CURVE

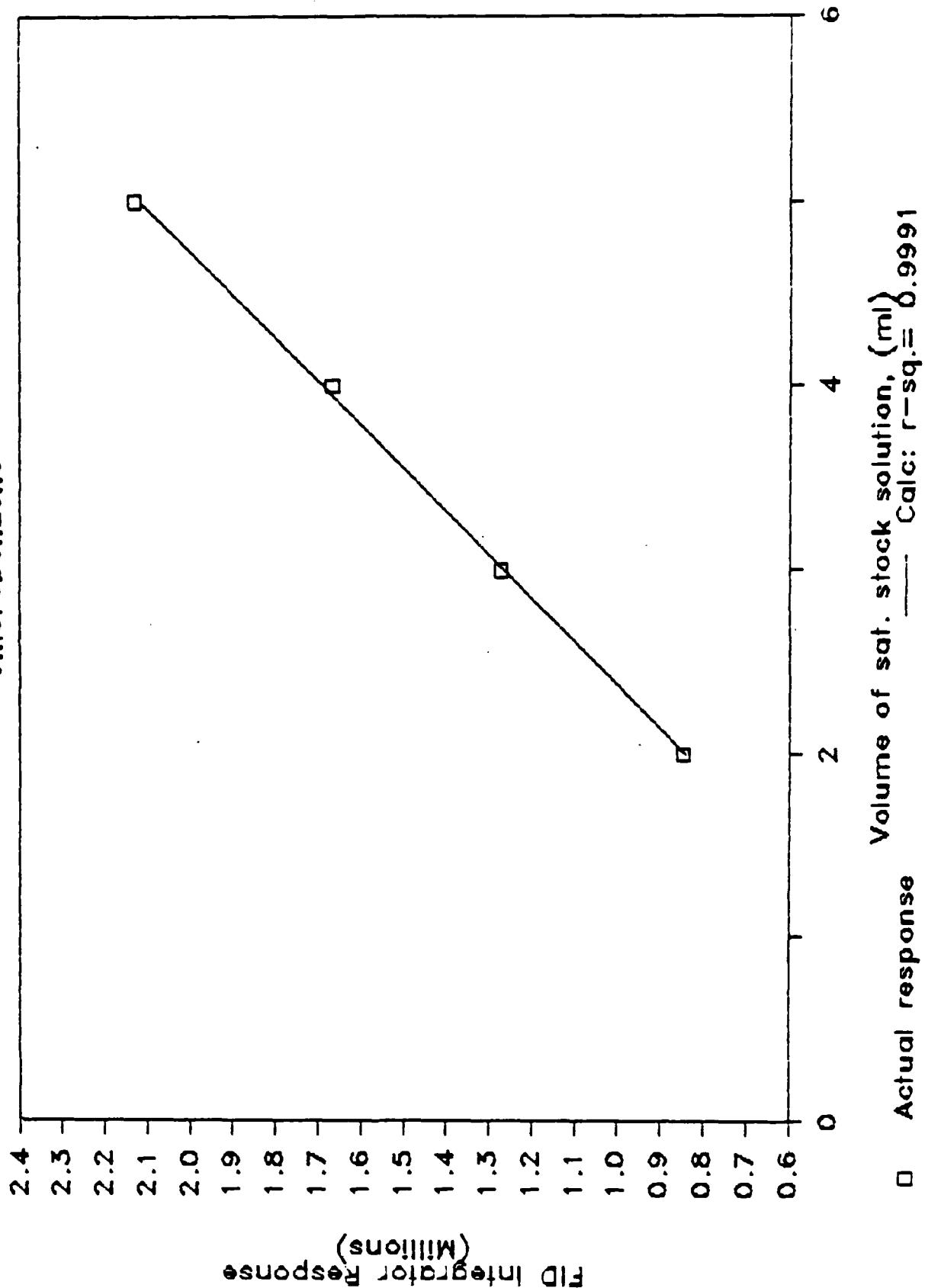
hexane



□ Actual response
— Calc: $r = \text{sq.} = 0.9984$

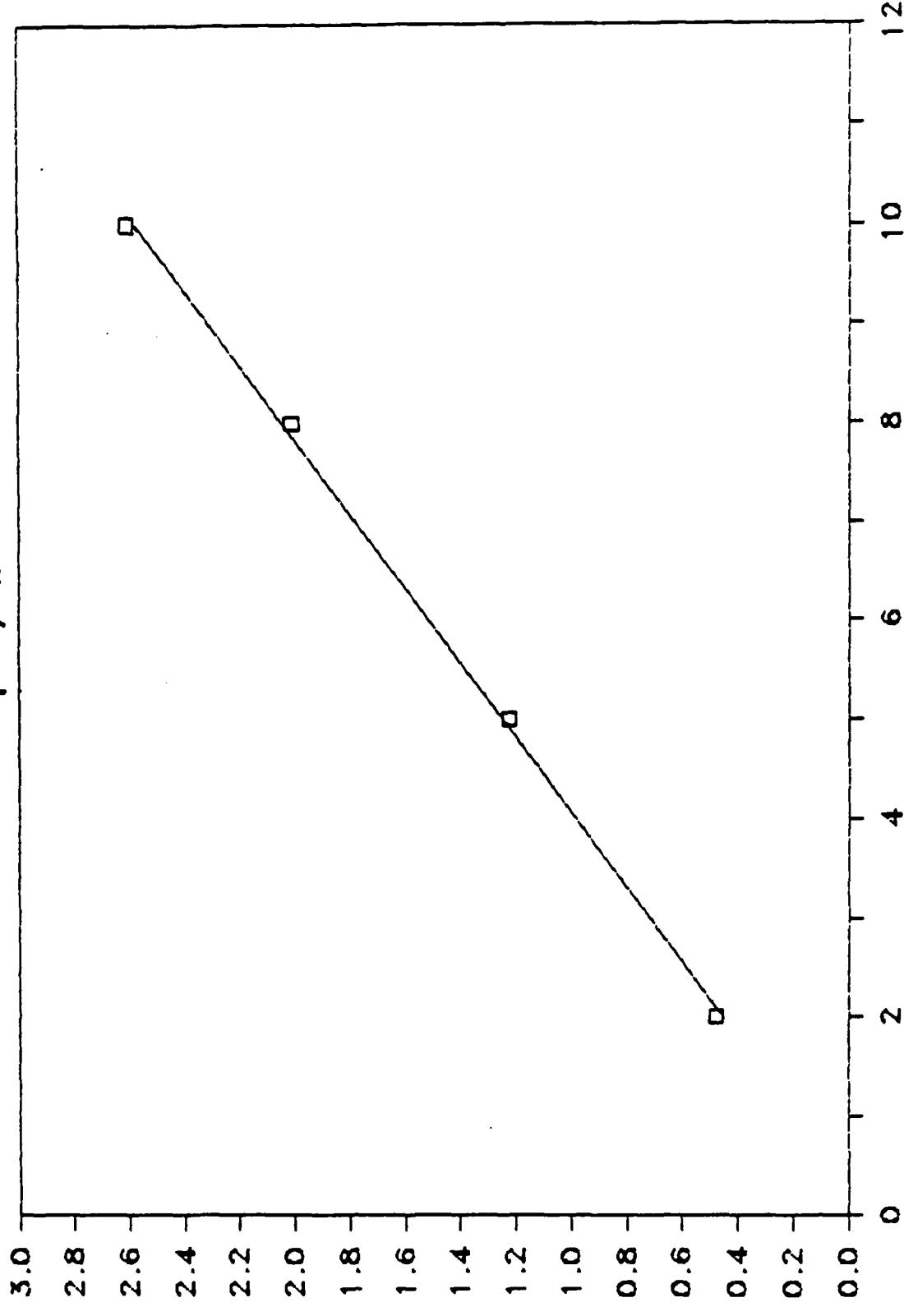
SERIAL DILUTION CURVE

Chlorobenzene



SERIAL DILUTION CURVE

p-Xylene

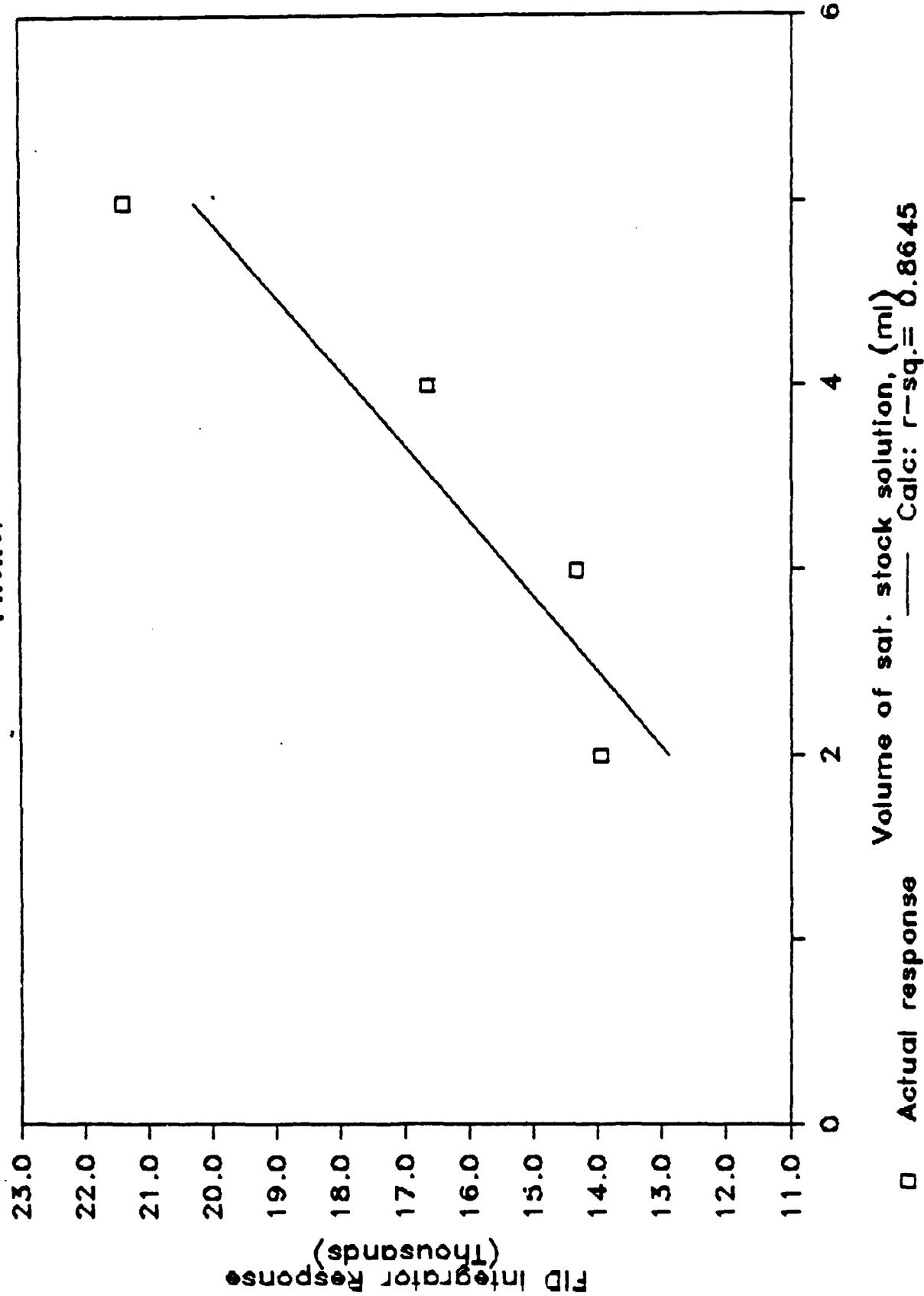


□ Actual response
Volume of sat. stock solution, (ml) Calc: $r = \frac{1}{2}x + 2.6$, $r^2 = 0.9987$

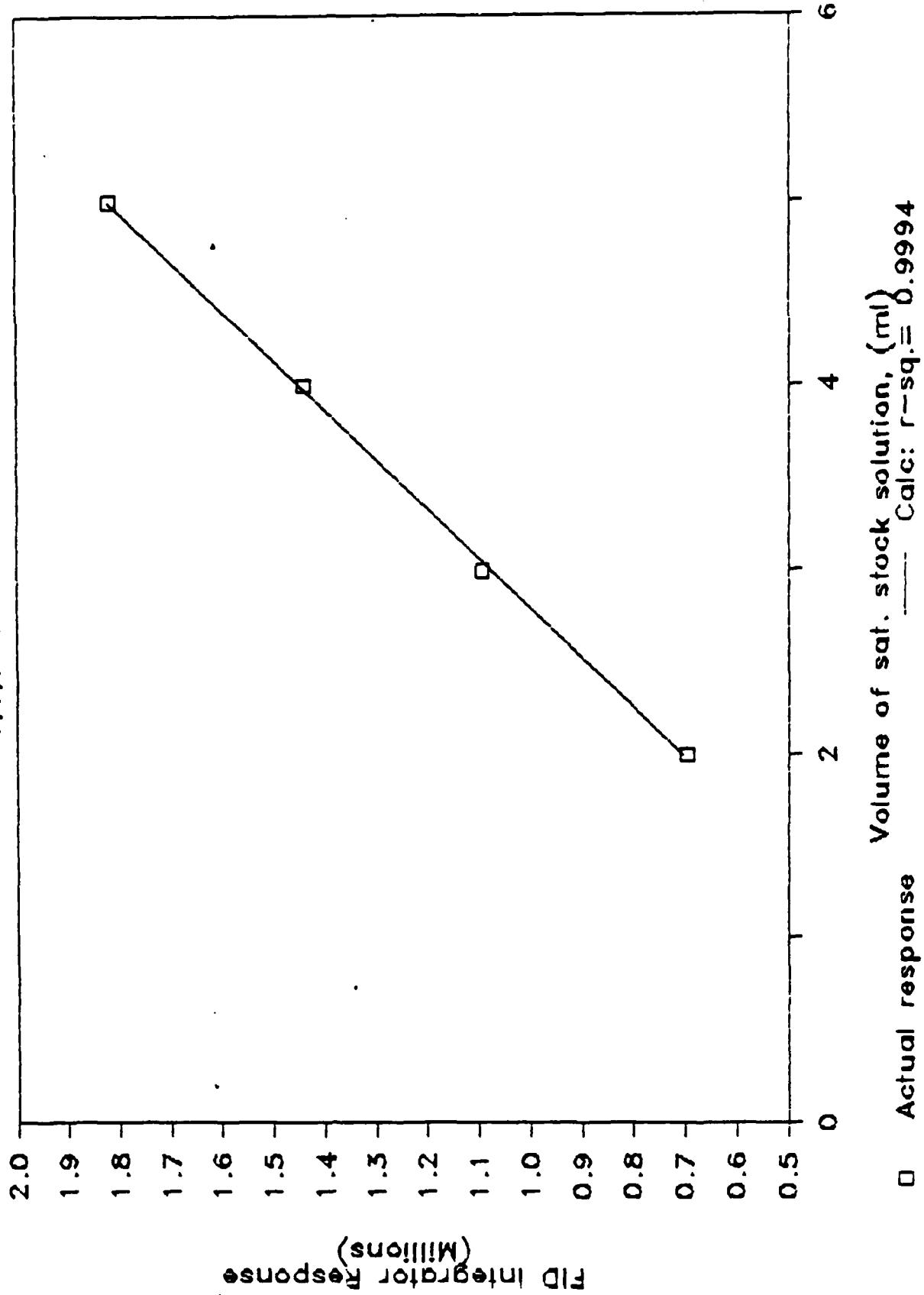
FID Integrator Response (Millions)

SERIAL DILUTION CURVE

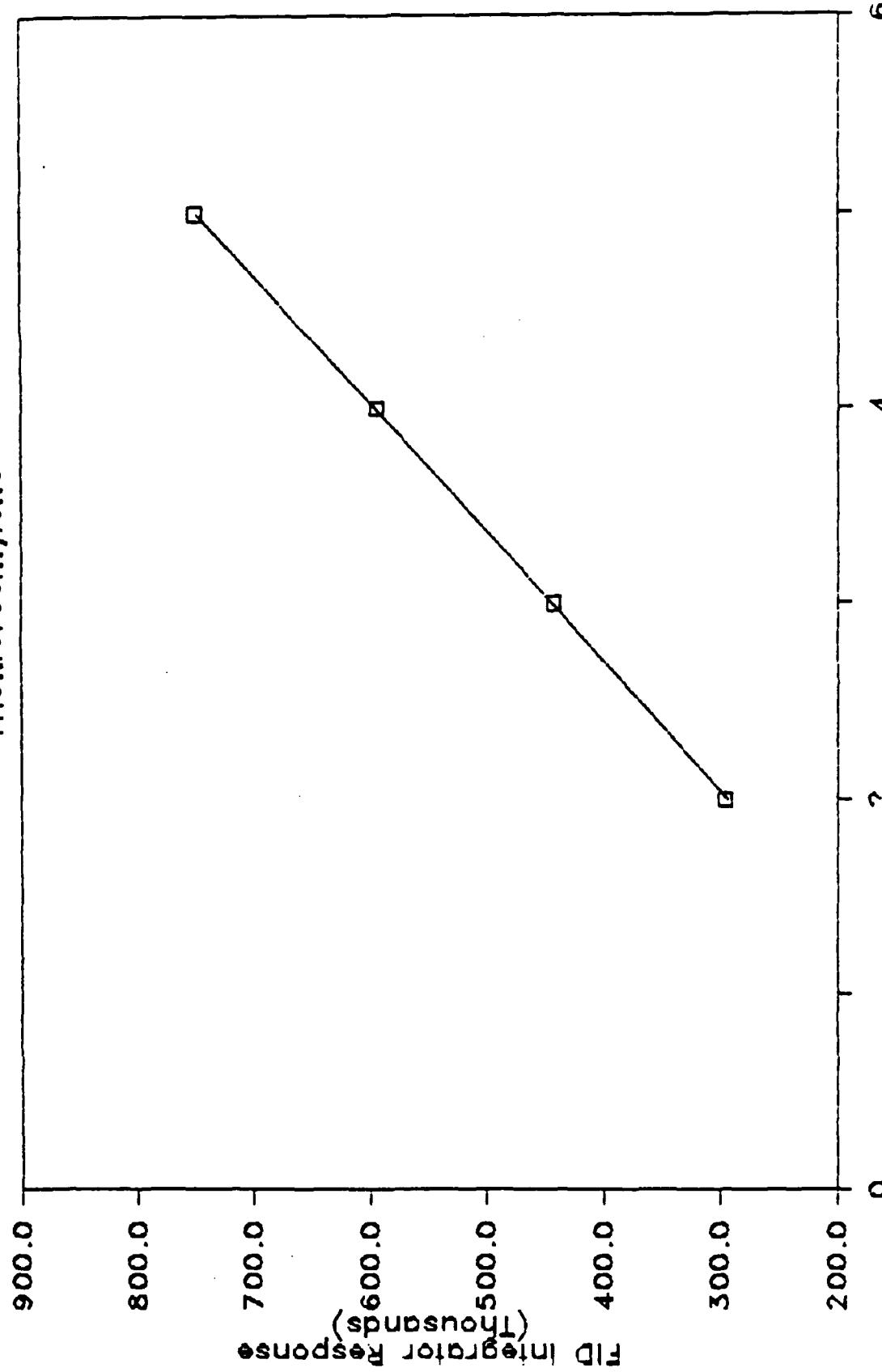
Phenol



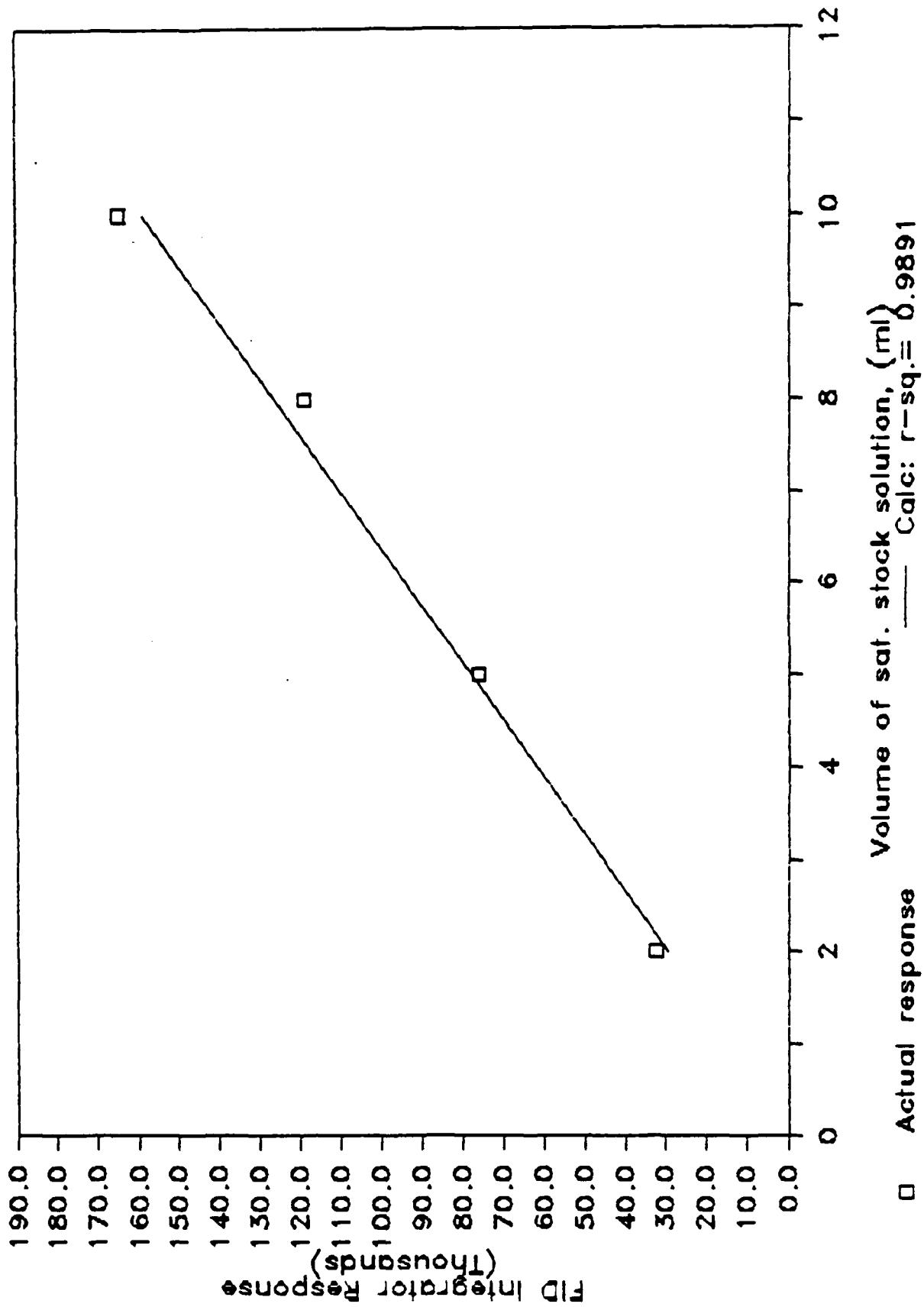
SERIAL DILUTION CURVE
1,1,1-Trichloroethane



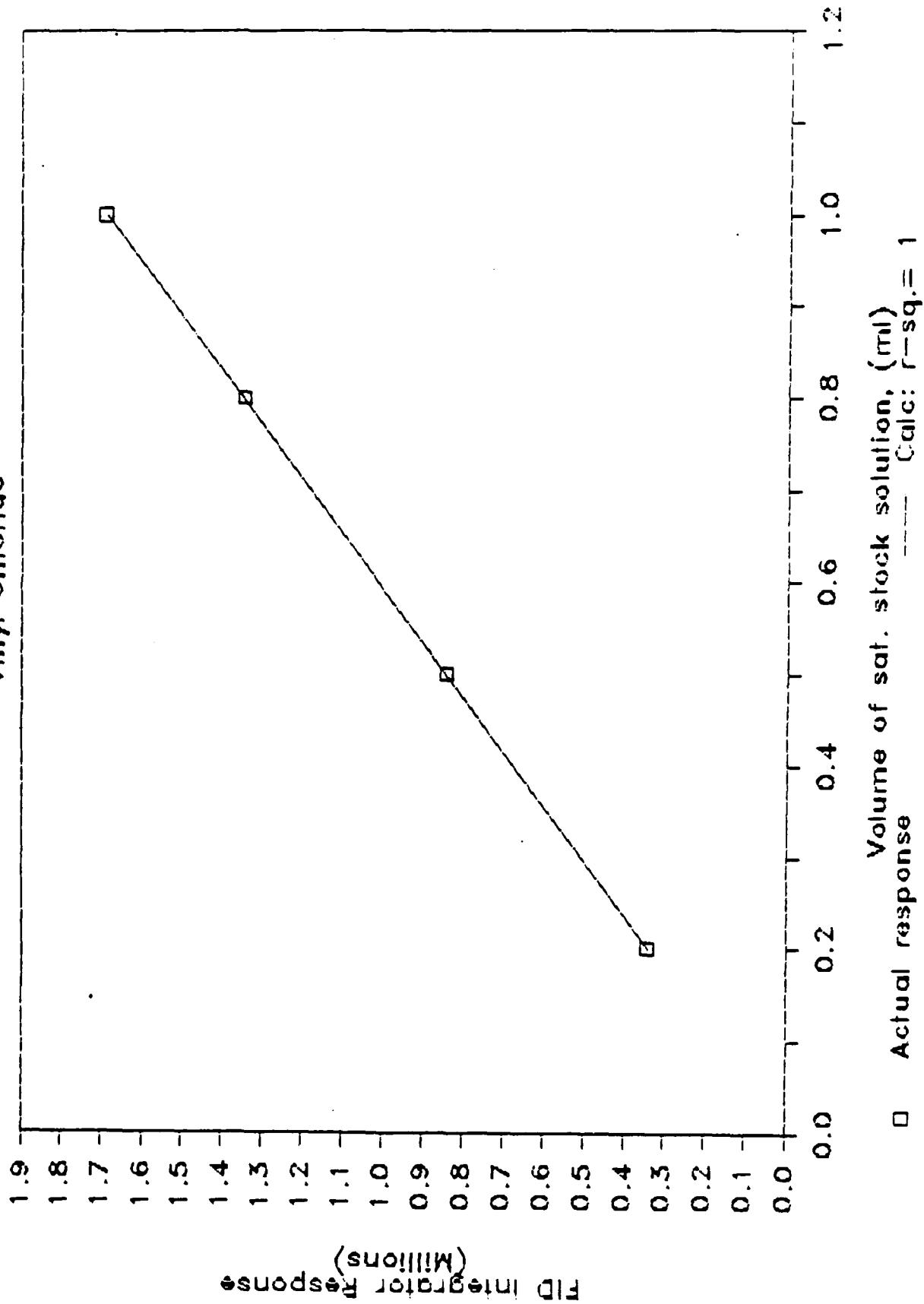
SERIAL DILUTION CURVE
Trichloroethylene



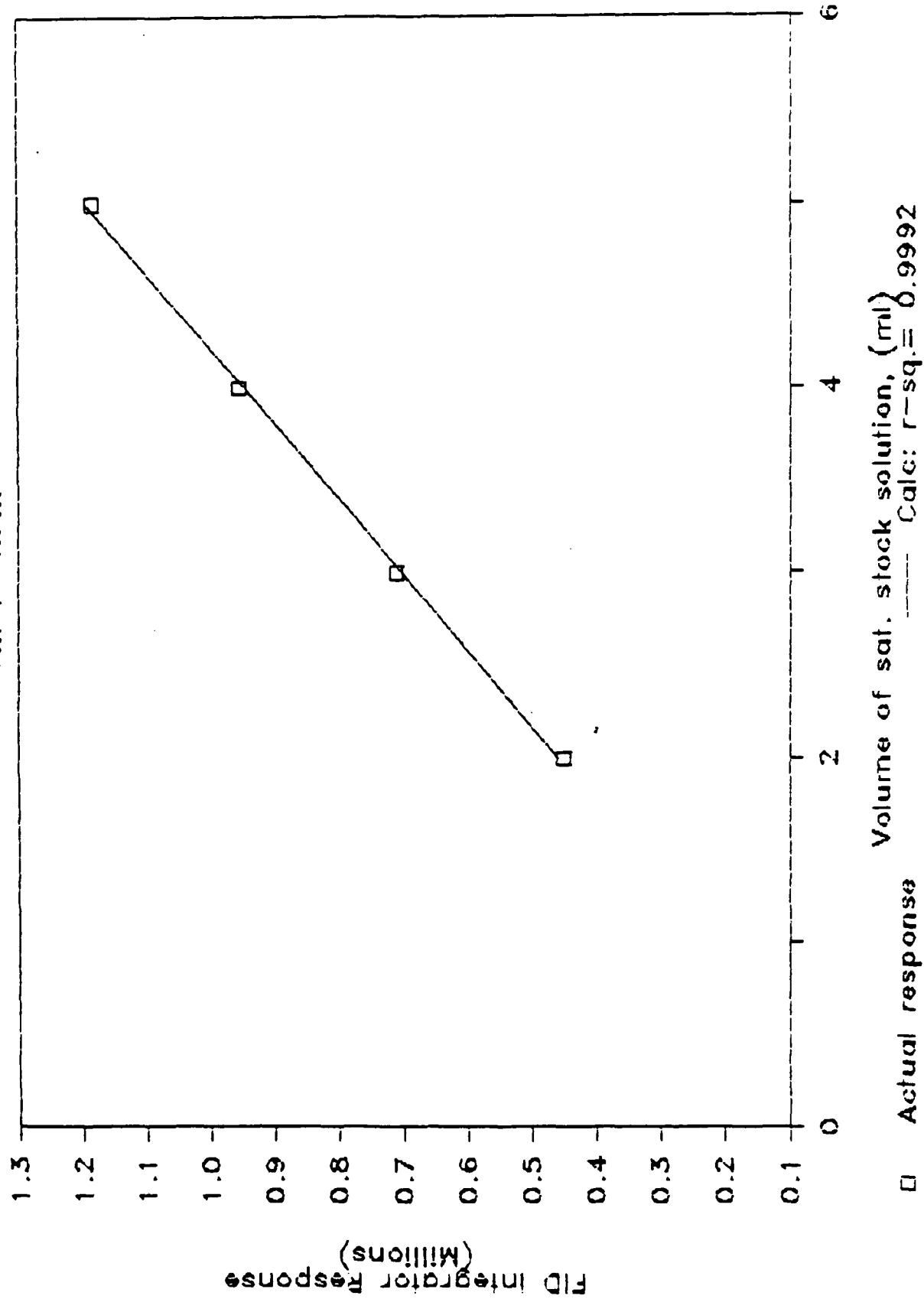
SERIAL DILUTION CURVE
Decalin



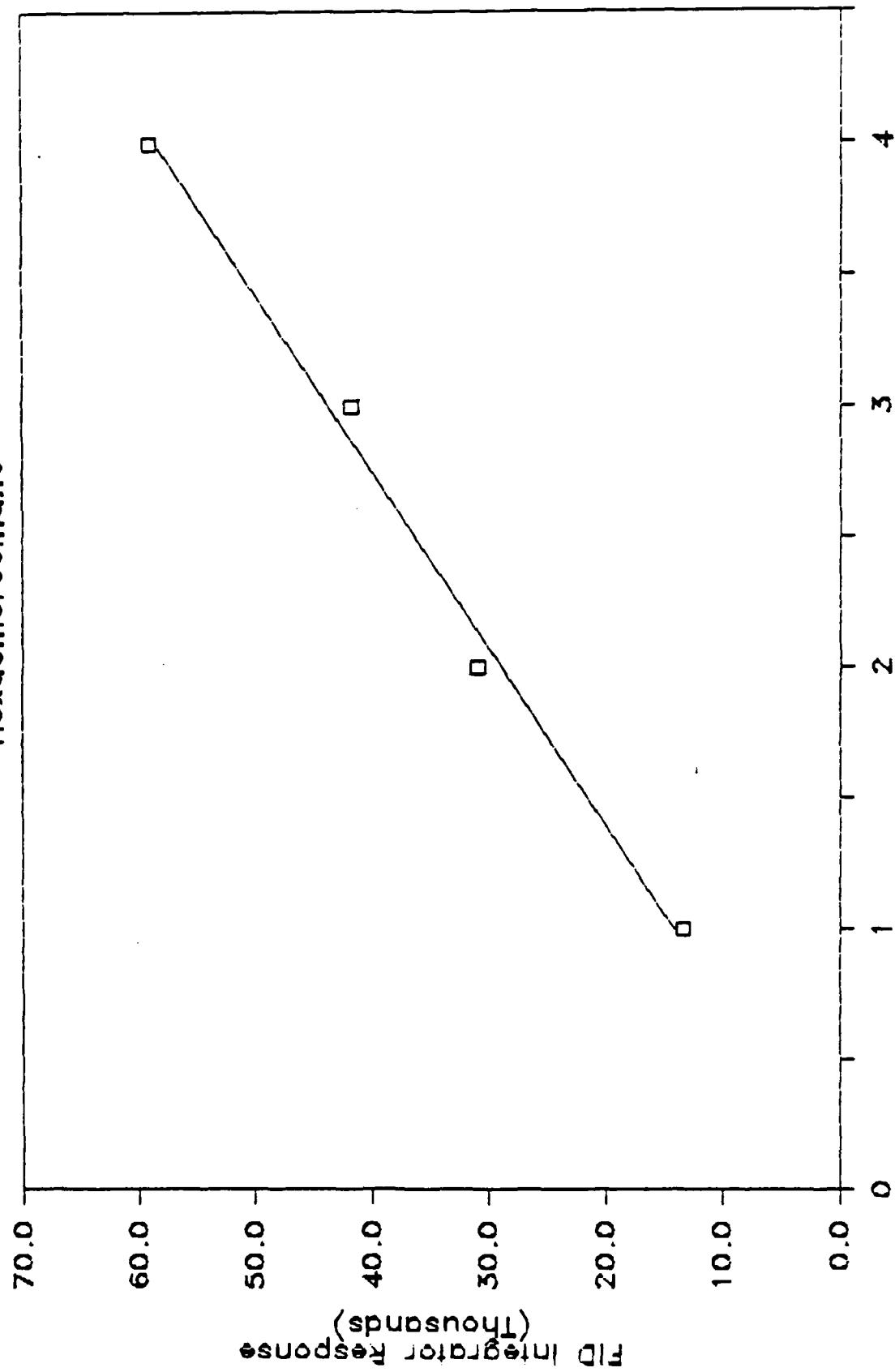
SERIAL DILUTION CURVE
Vinyl Chloride



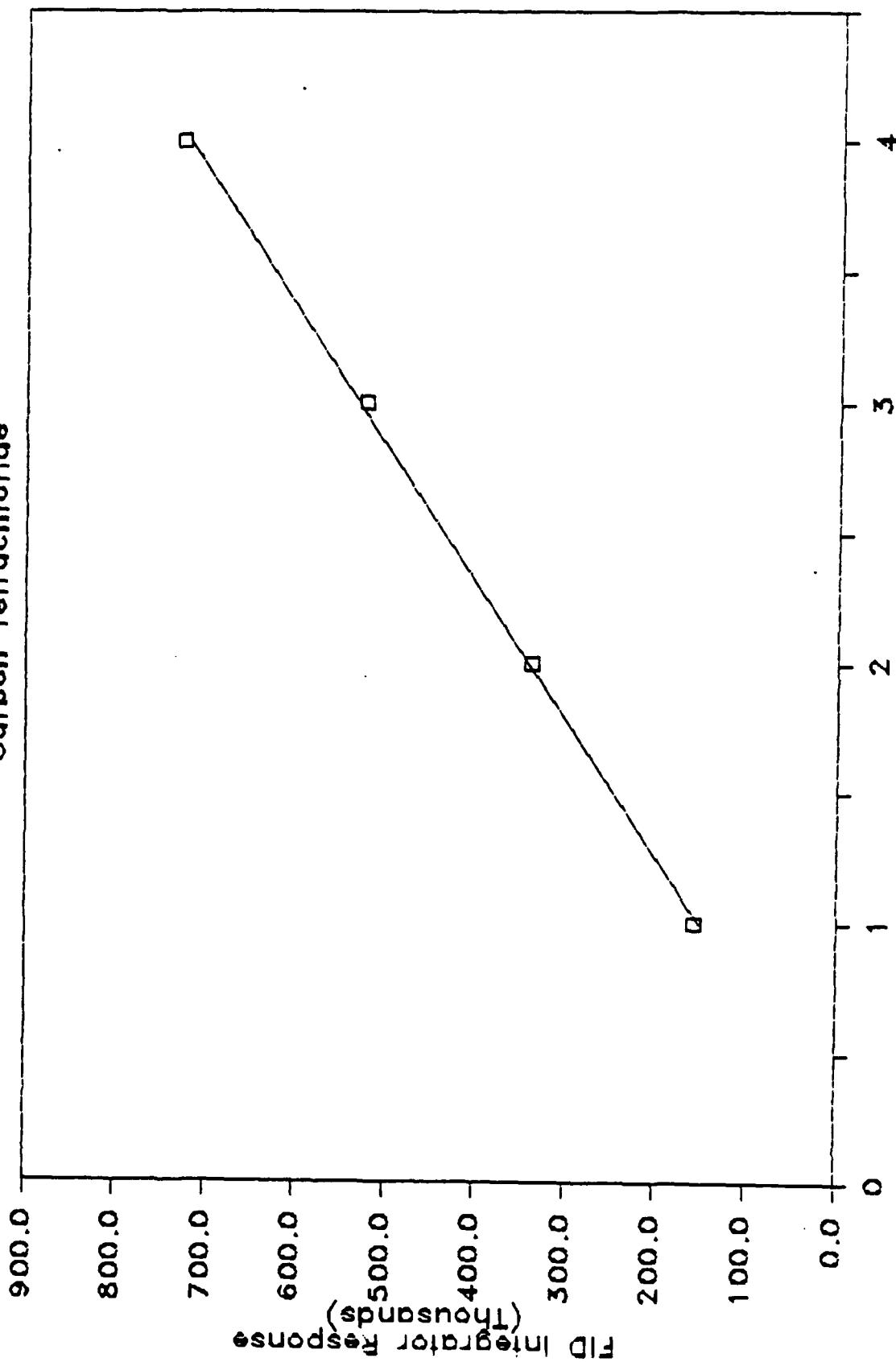
SERIAL DILUTION CURVE
Chloroethane



SERIAL DILUTION CURVE
Hexachloroethane



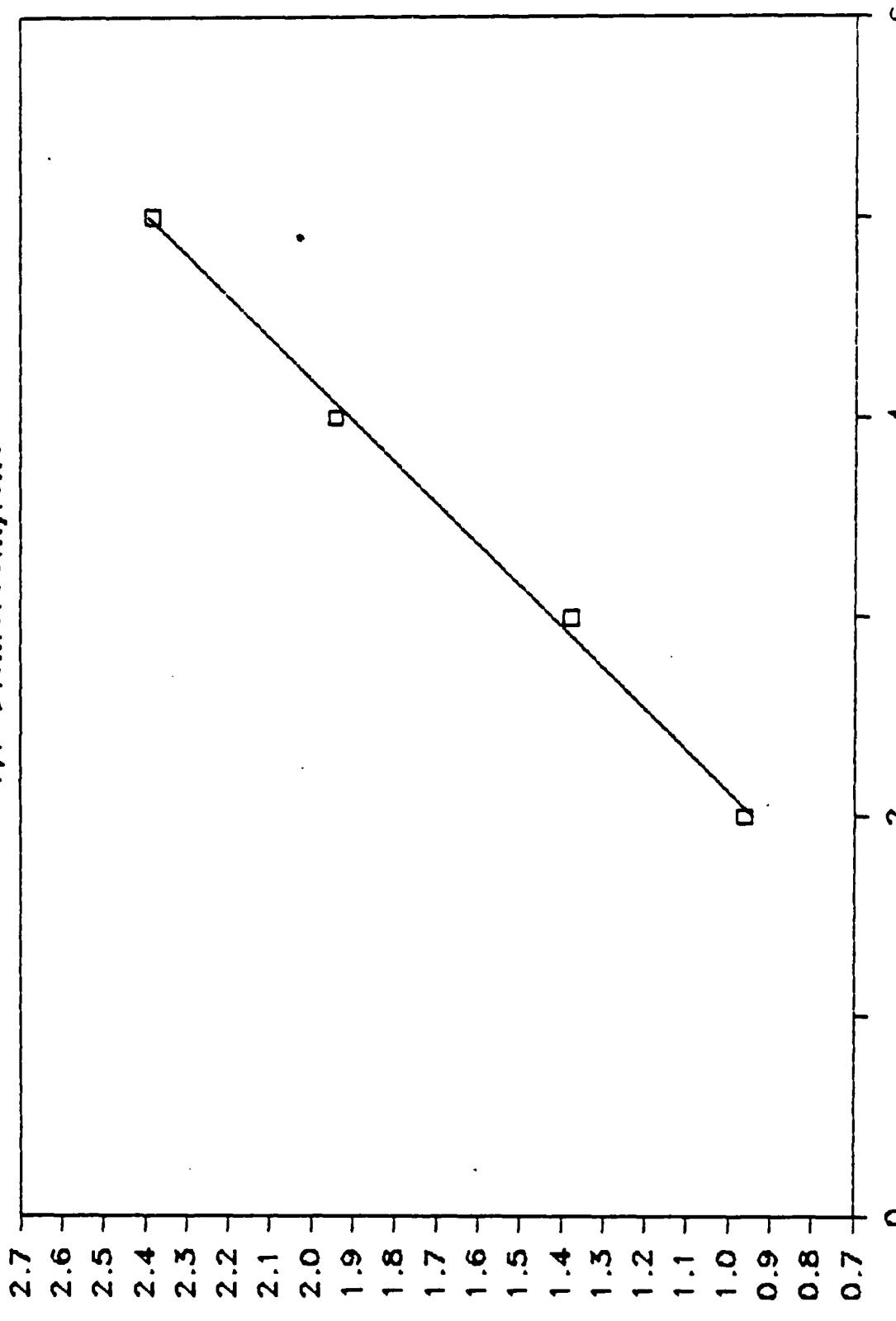
SERIAL DILUTION CURVE
Carbon Tetrachloride



□ Actual response — Calc: $r = \text{sq. root of } 0.9992$

SERIAL DILUTION CURVE

1,1-Dichloroethylene

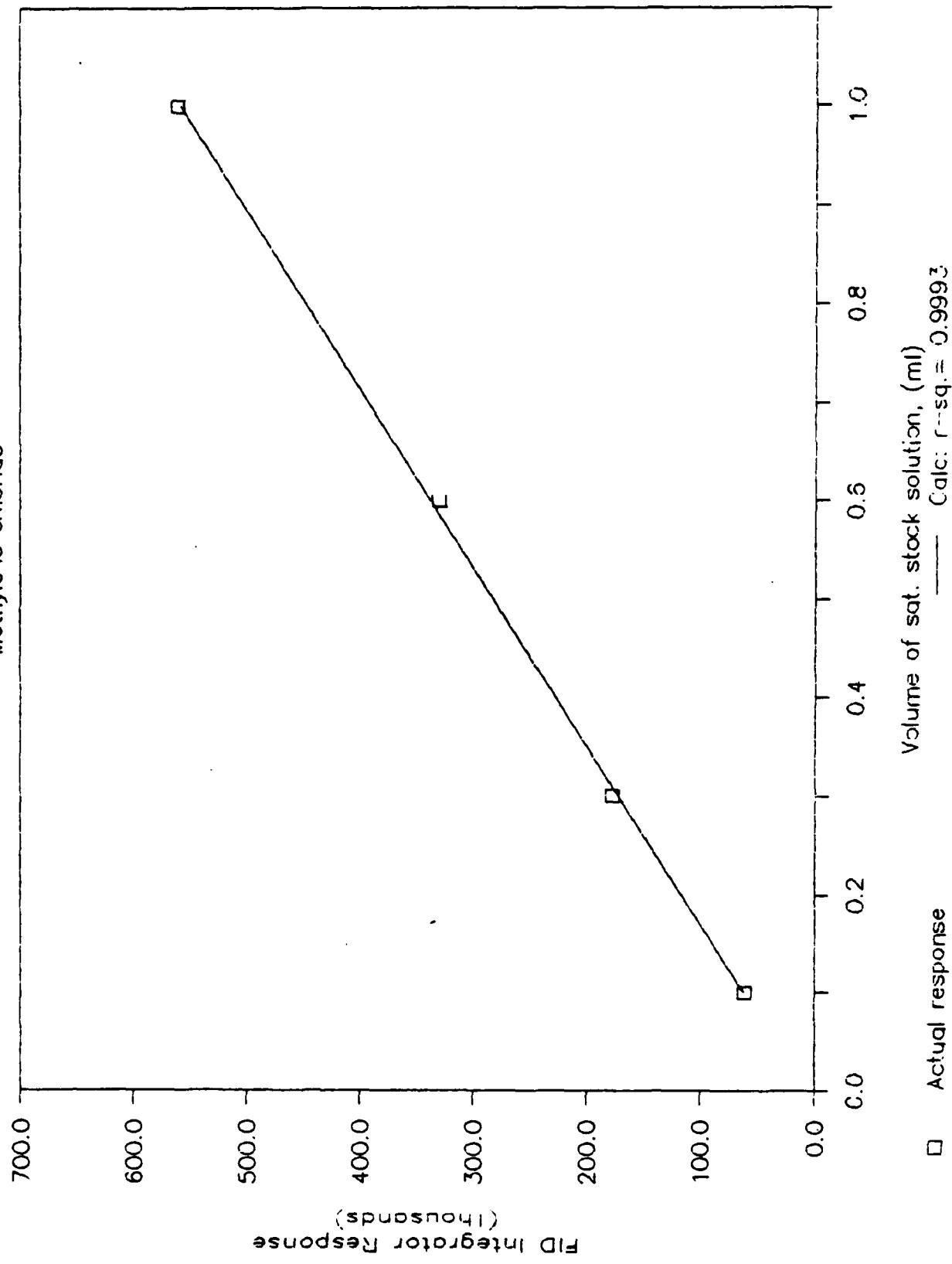


FID Integrator Response
(Millions)

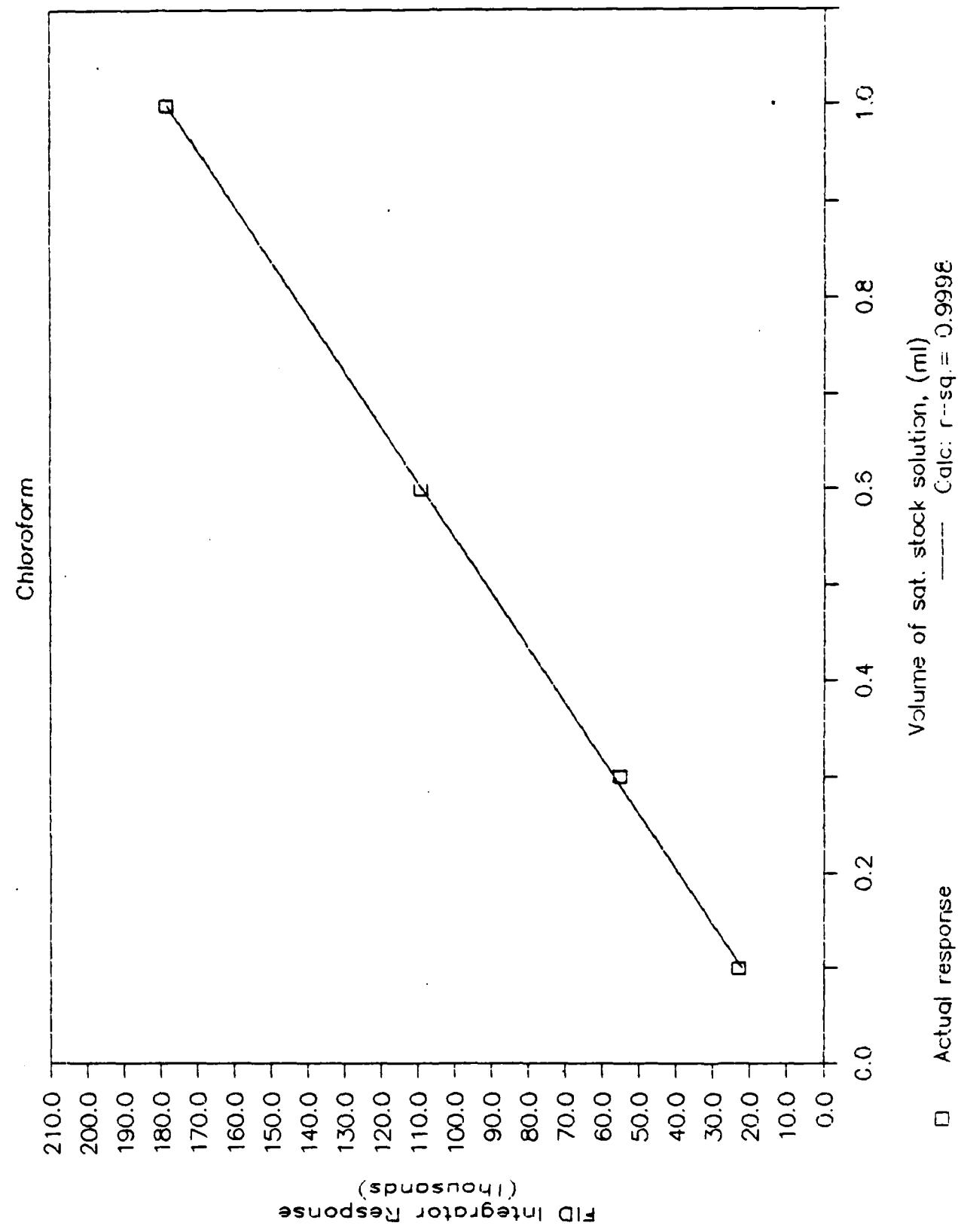
□ Actual response Volume of sat. stock solution, (ml)
Calc: $r - \text{sq.} = 0.9967$

SERIAL DILUTION CURVE

Methylene chloride

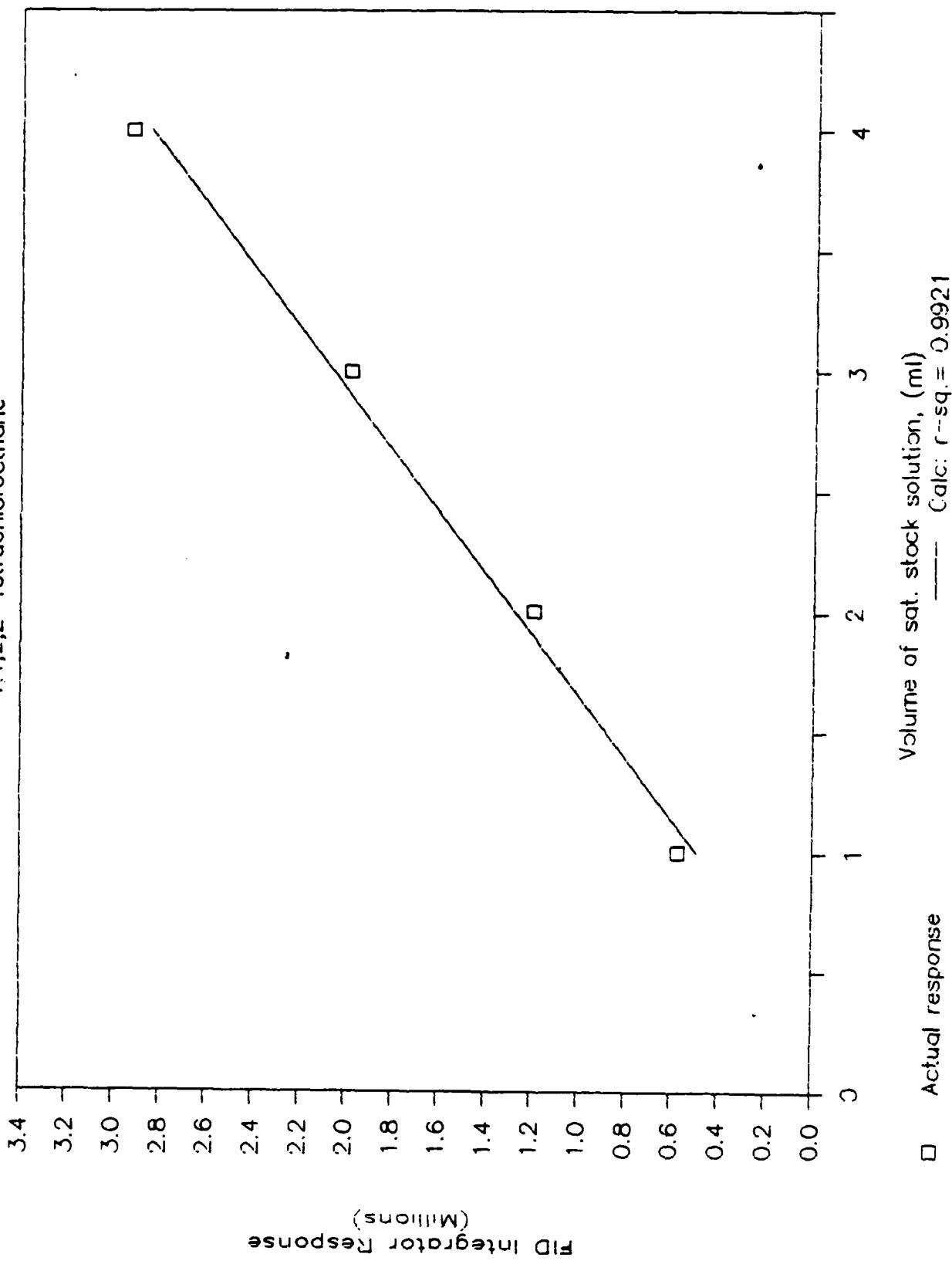


SERIAL DILUTION CURVE



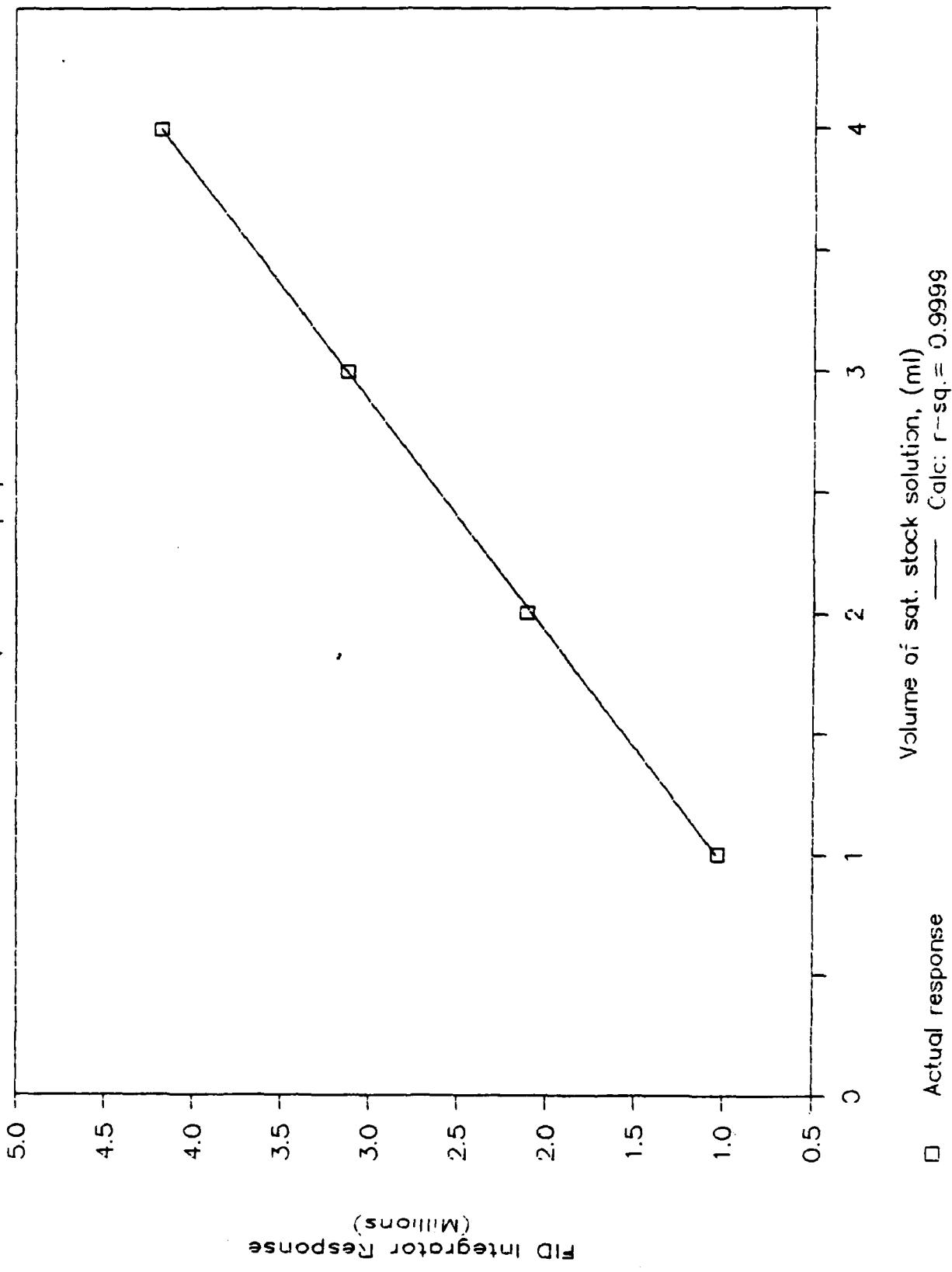
SERIAL DILUTION CURVE

1,1,2,2-Tetrachloroethane



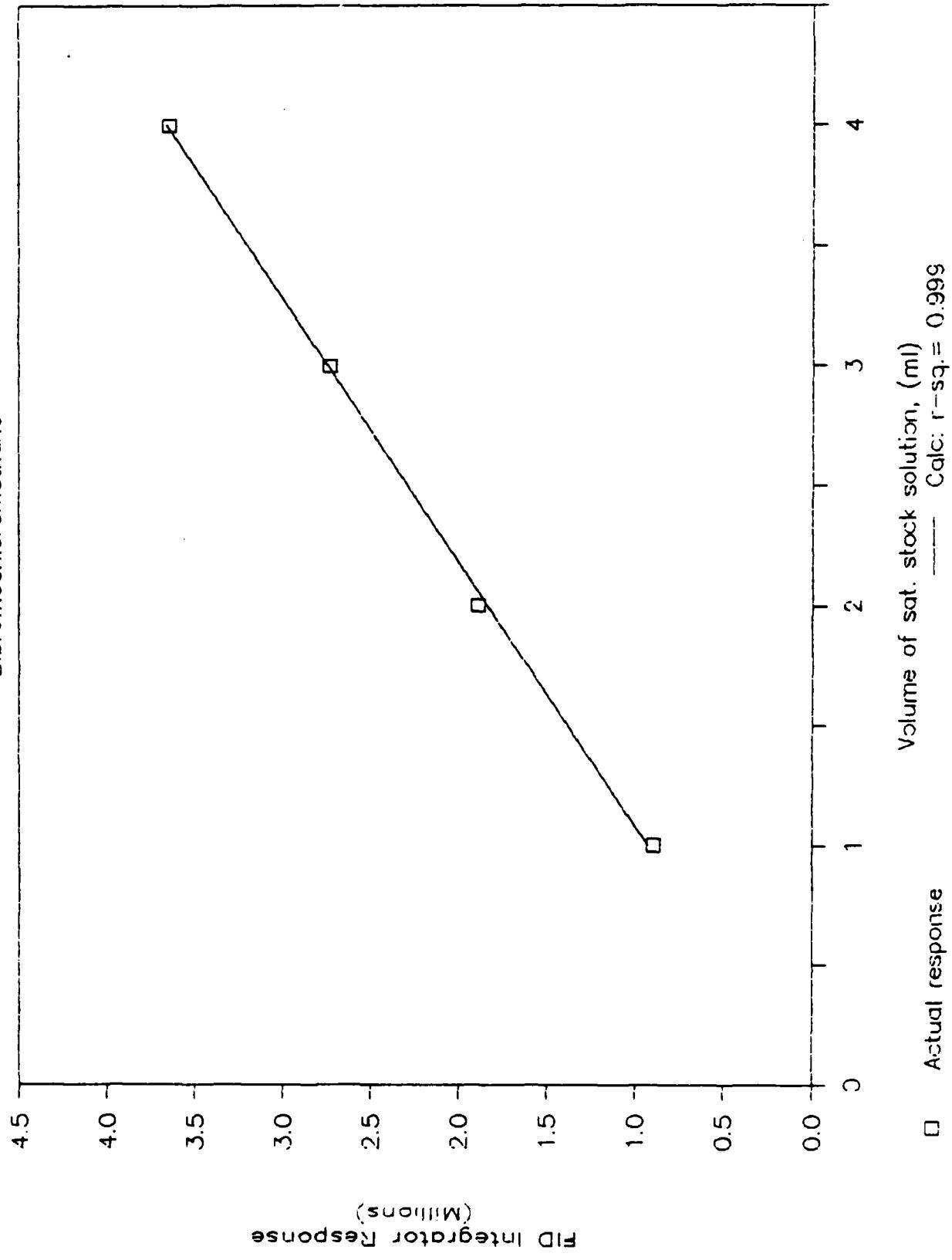
SERIAL DILUTION CURVE

1,2-Dichloropropane



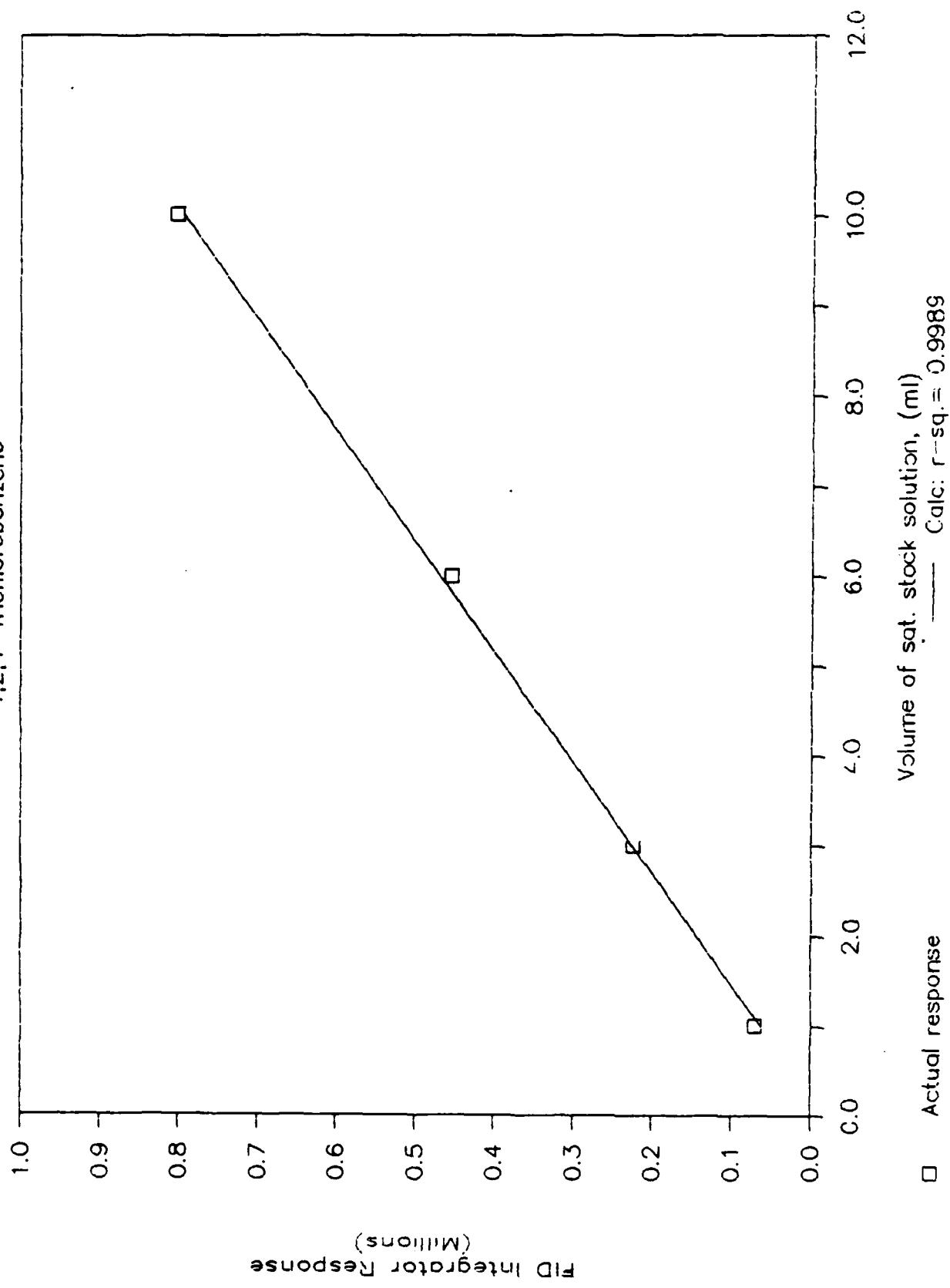
SERIAL DILUTION CURVE

Dibromochloromethane



SERIAL DILUTION CURVE

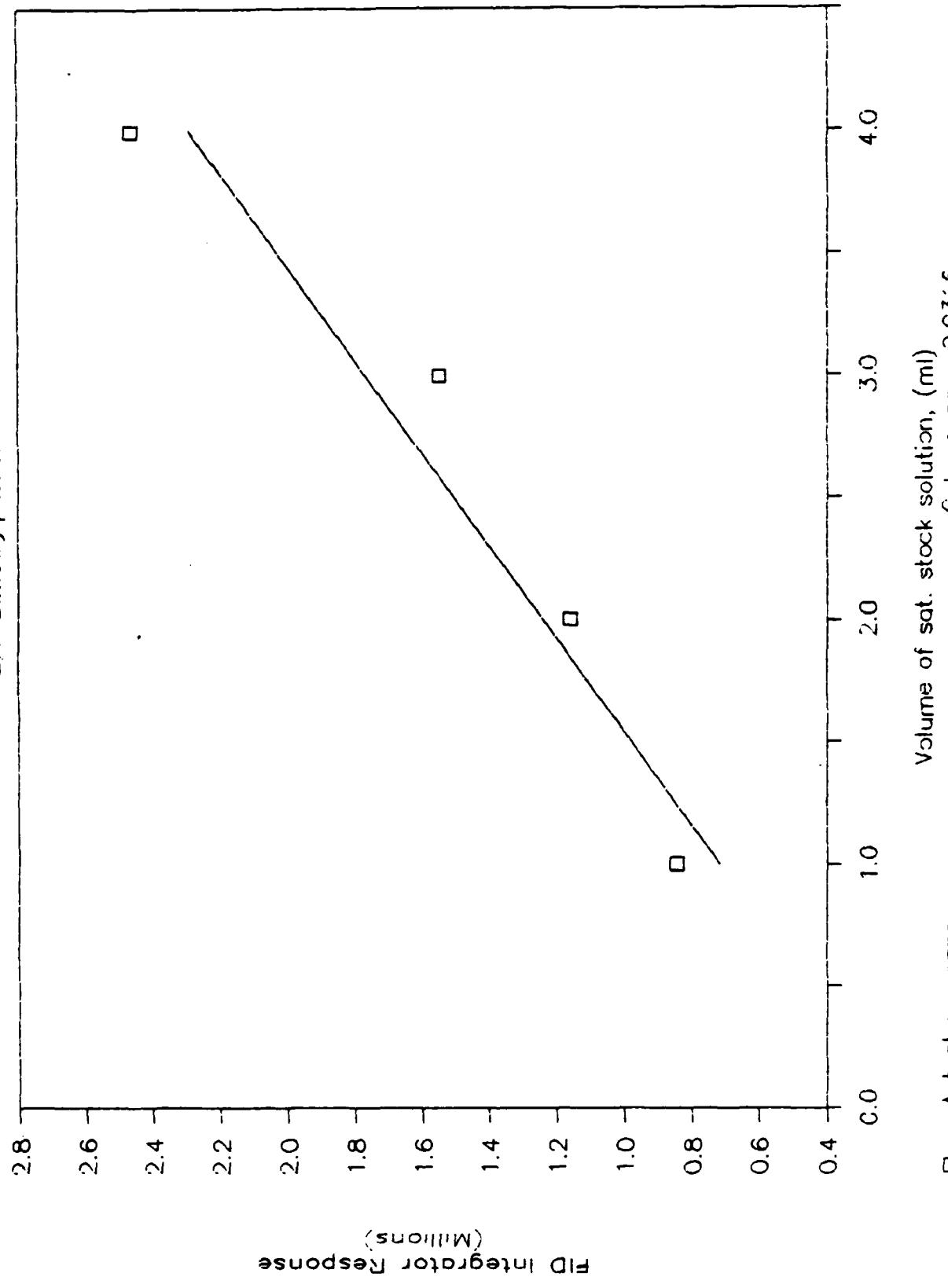
1,2,4-Trichlorobenzene



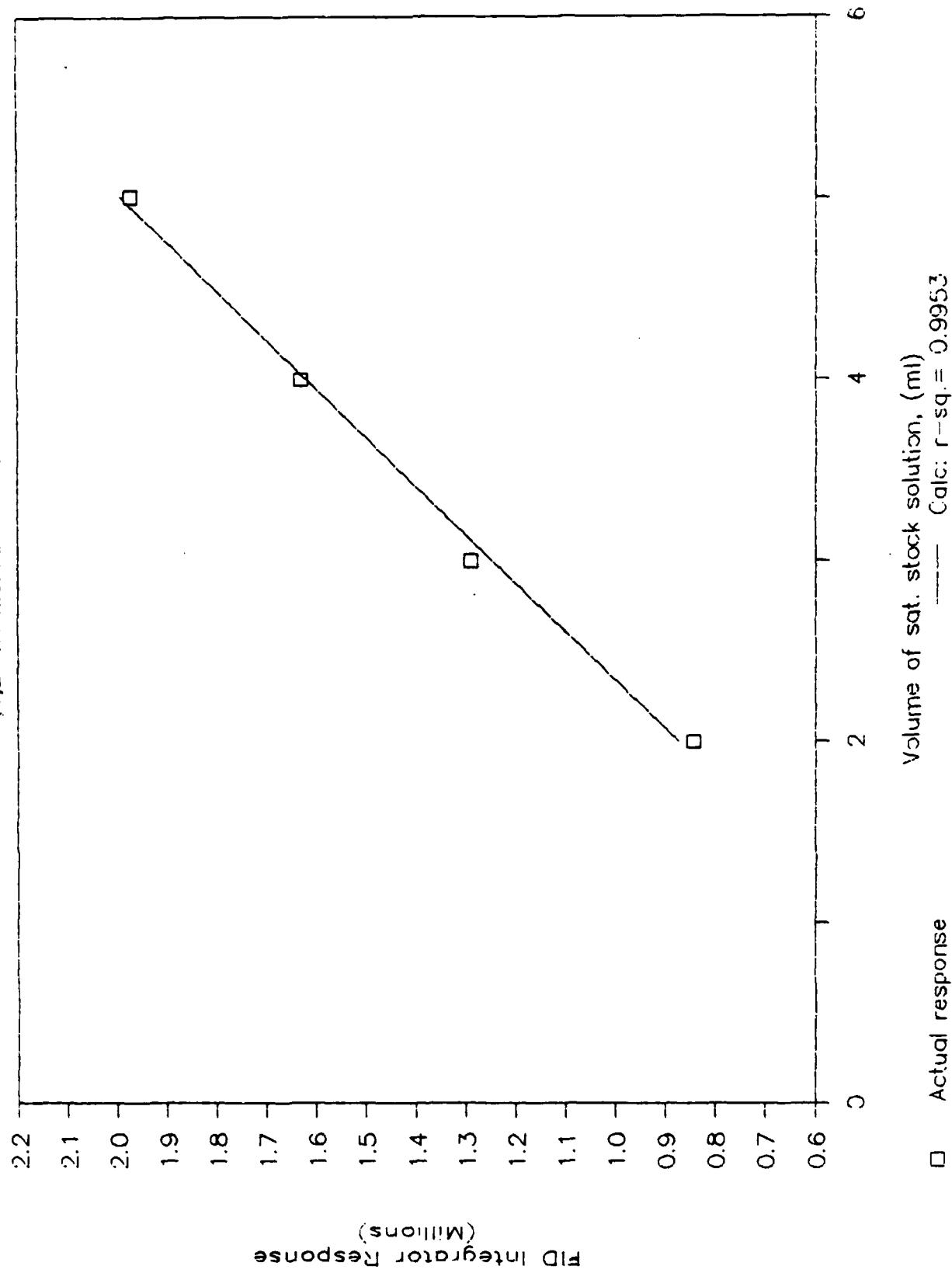
FID Integrator Response
(Millions)

SERIAL DILUTION CURVE

2,4-Dimethylphenol

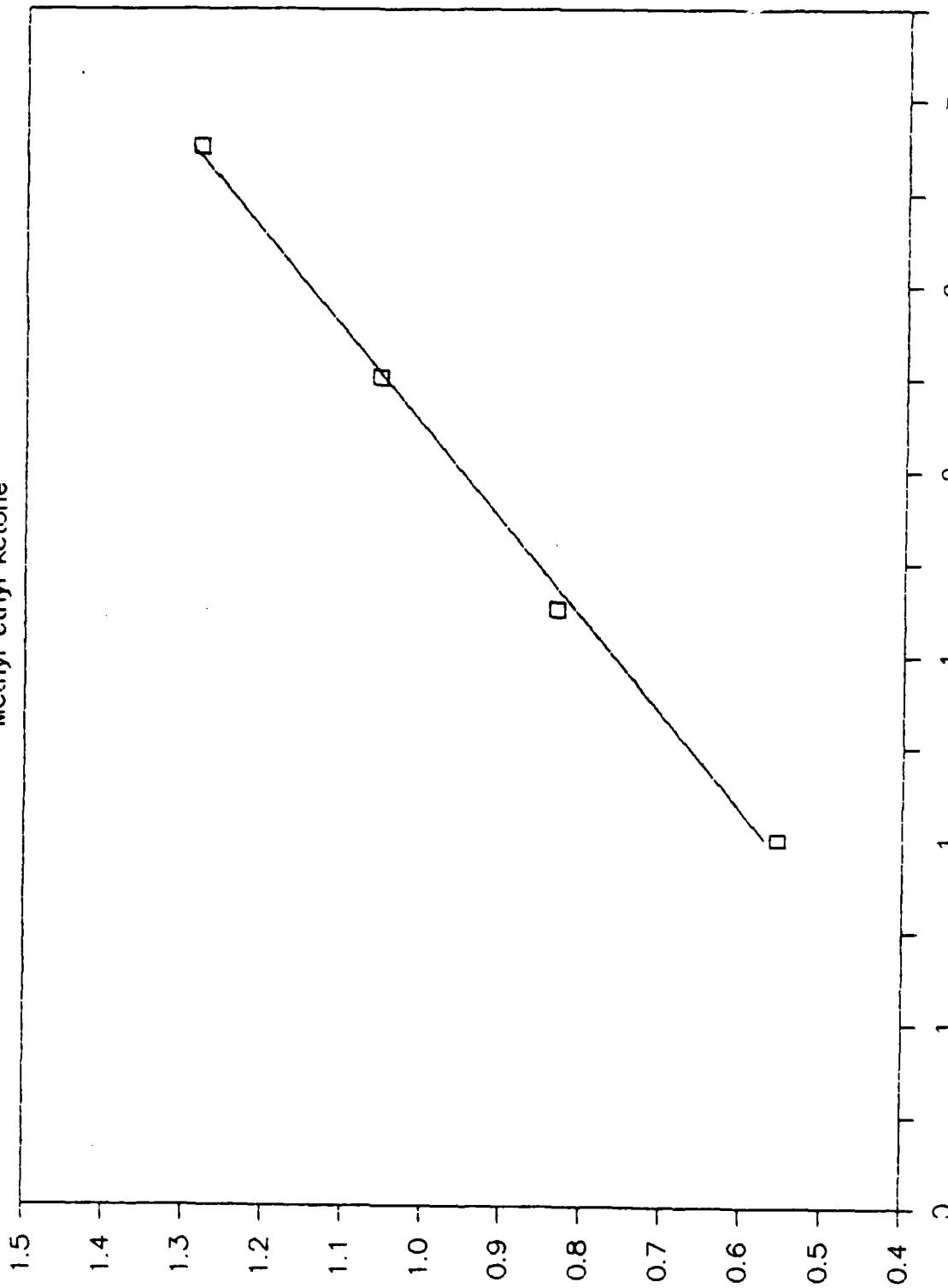


SERIAL DILUTION CURVE
1,1,2-Trichlorotrifluoroethane



SERIAL DILUTION CURVE

Methyl ethyl ketone

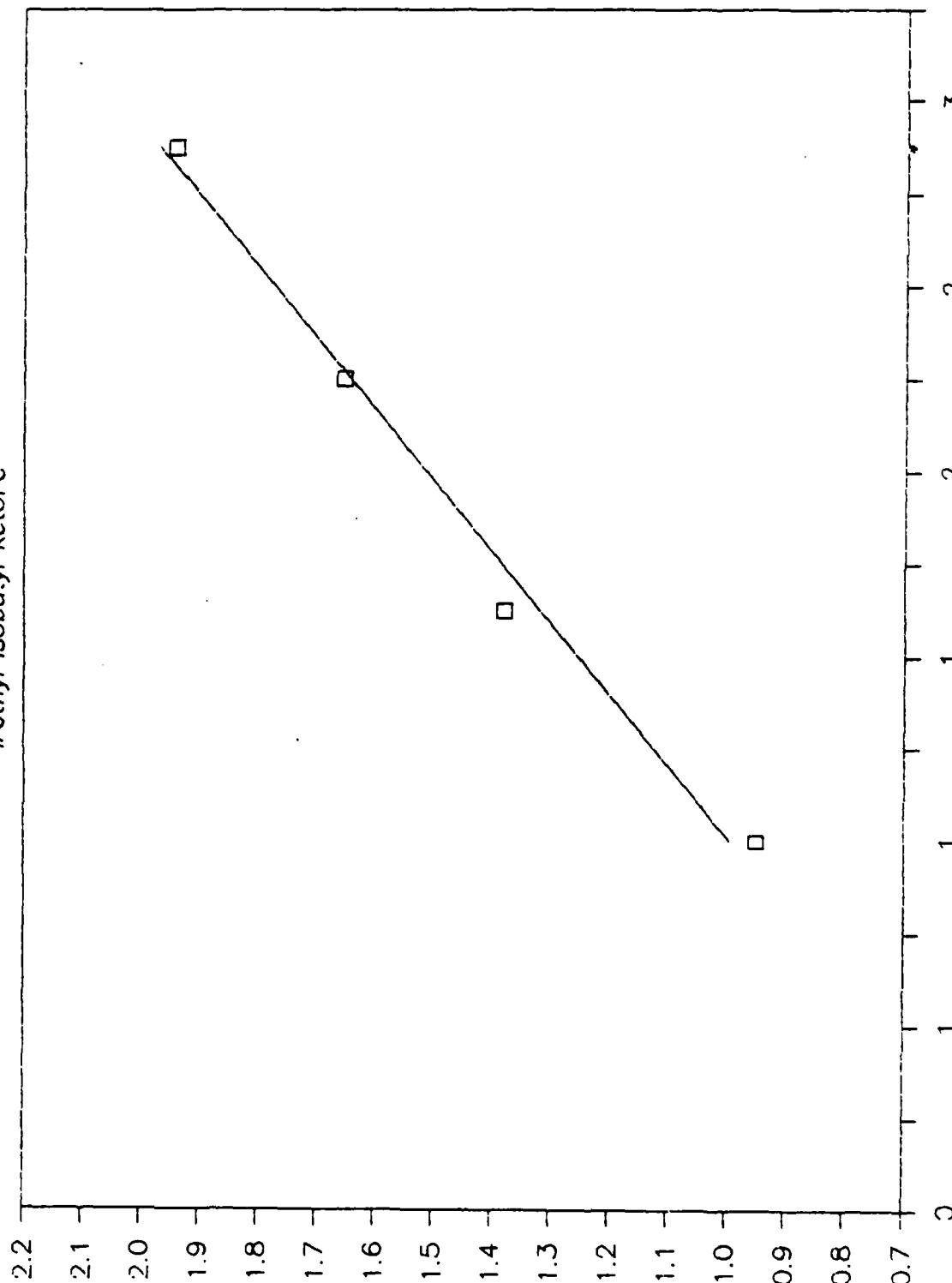


□ Actual response
Calc: $r = \text{sq.} = 0.997$

TID Integrator Response
(Millions)

SERIAL DILUTION CURVE

Methyl isobutyl ketone



□ Actual response

Volume of sat. stock solution, (ml)
Calc: $r = \text{sq.} = 0.9878$

FID integrator Response
(Millions)

Component Data

06-Nov-86

Results Summary for Component 1

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	2	2	2	2	3	3
REPLICATE →	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	1		1		1	
Component ID	1		1		1	
Temperature (C)	10		15		20	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H _{avg} : atm-m ³ /mol	14.4468	1.0E-25	16.6177	1.0E-25	32.7919	1.0E-25
H _{avg} : atm-mol/mol	18631.0		21818.3		43785.5	
H _{avg} : atm-m ³ /mol	3.36E-01	1	3.93E-01	1	7.89E-01	1
H _{avg} : kPa-m ³ /mol	34.8184		39.8141		79.9291	
COV, r [std/mean]	15.59		19.64		62.96	
COV, both replic.	_____		_____		_____	
Observation: (1)	13.8845		13.6479		37.1622	
[atm-m ³ /mol] (2)	17.3798		13.9520		60.1730	
(3)	11.9408		19.1588		15.1897	
(4)	14.5788		19.7121		18.6428	
Injection: (1)	161500		259600		306200	
[Peak Area] (2)	154040		281430		261140	
(3)	40073		64730		63322	
(4)	37936		64352		60409	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		3		3	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		1		1	
Component ID		1		1	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H _{avg} : atm-m ³ /m ³		19.7111	1.0E-25	33.6200	1.0E-25
H _{avg} : atm-mol/mol		26768.1		46422.5	
H _{avg} : atm-m ³ /mol		4.82E-01	1	8.35E-01	1
H _{avg} : kPa-m ³ /mol		48.8644		84.7429	
COV, r [std/mean]		22.13		61.56	
COV, both replic.		_____		_____	
Observations: (1)		22.2479		50.5776	
[atm-m ³ /m ³] (2)		24.5110		52.4824	
(3)		15.4631		15.6022	
(4)		16.6222		15.8179	
Injection: (1)		180140		449010	
[Peak Area] (2)		166650		373870	
(3)		48235		89870	
(4)		39548		89572	

Temperature Regression Parameters:

OF POINTS = 5

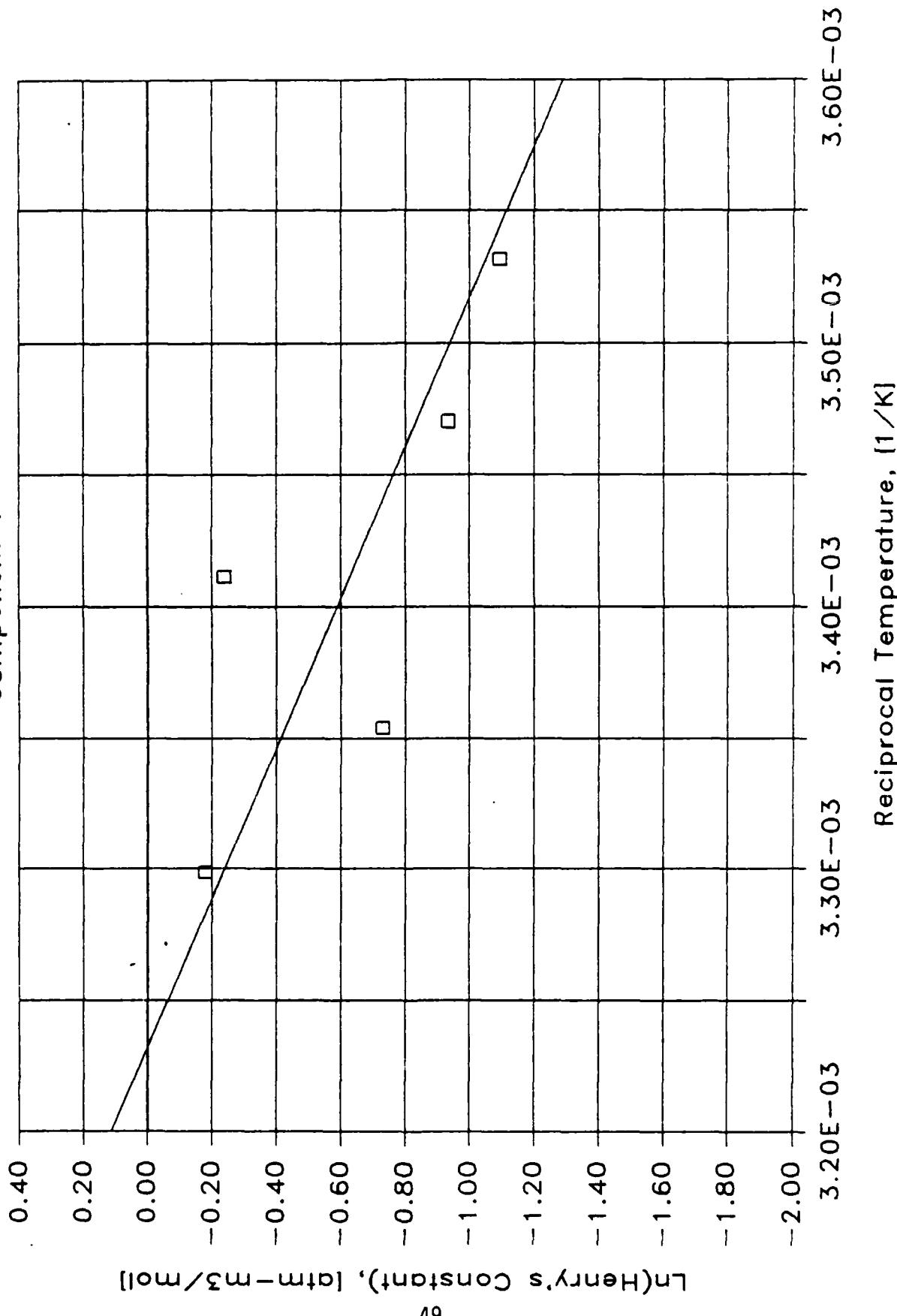
SLOPE = -3.5E+03

Y-INTERCEPT = 1.1E+01

R-SQUARED = 0.6165

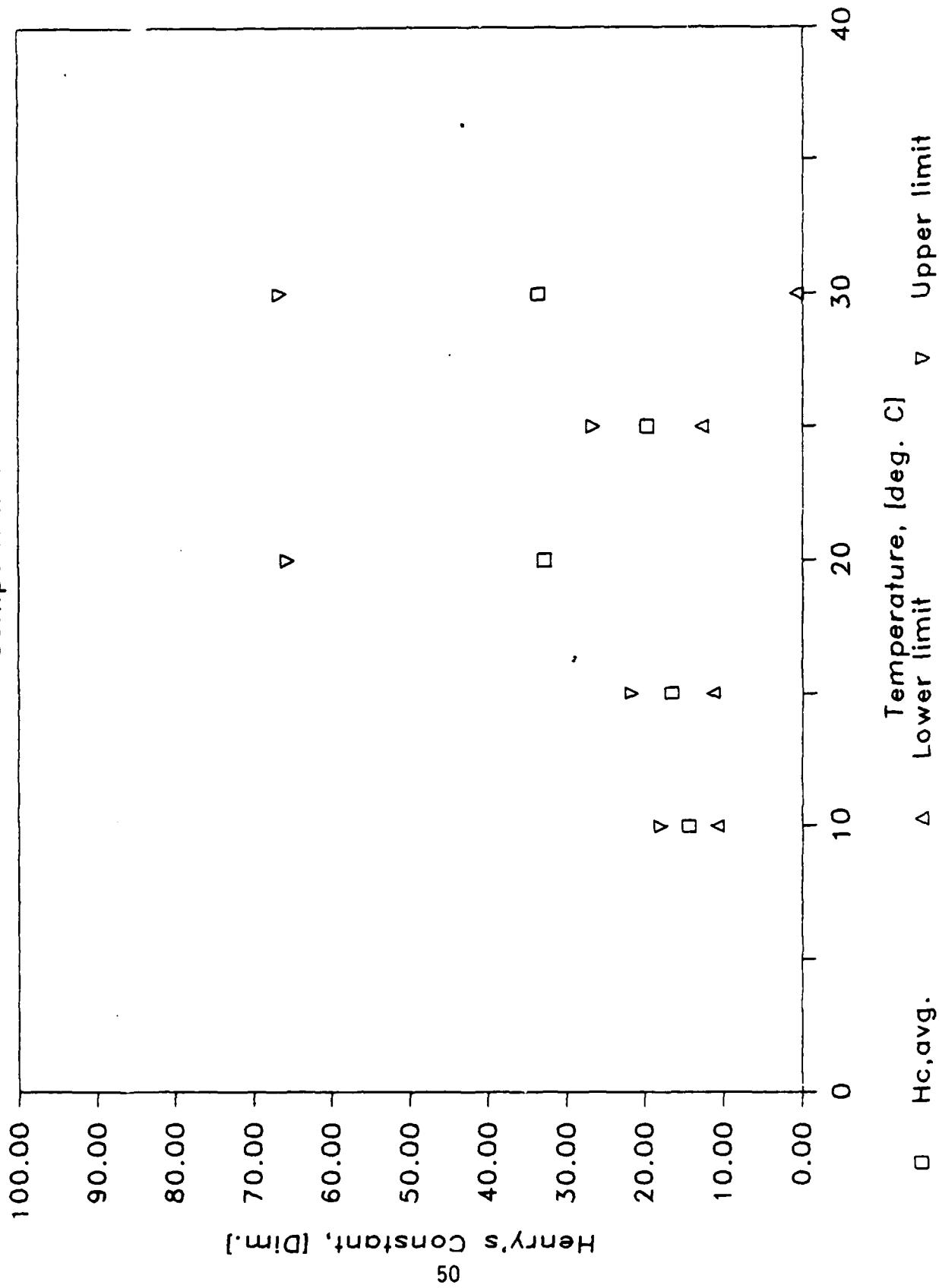
TEMPERATURE REGRESSION PLOT

Component 1



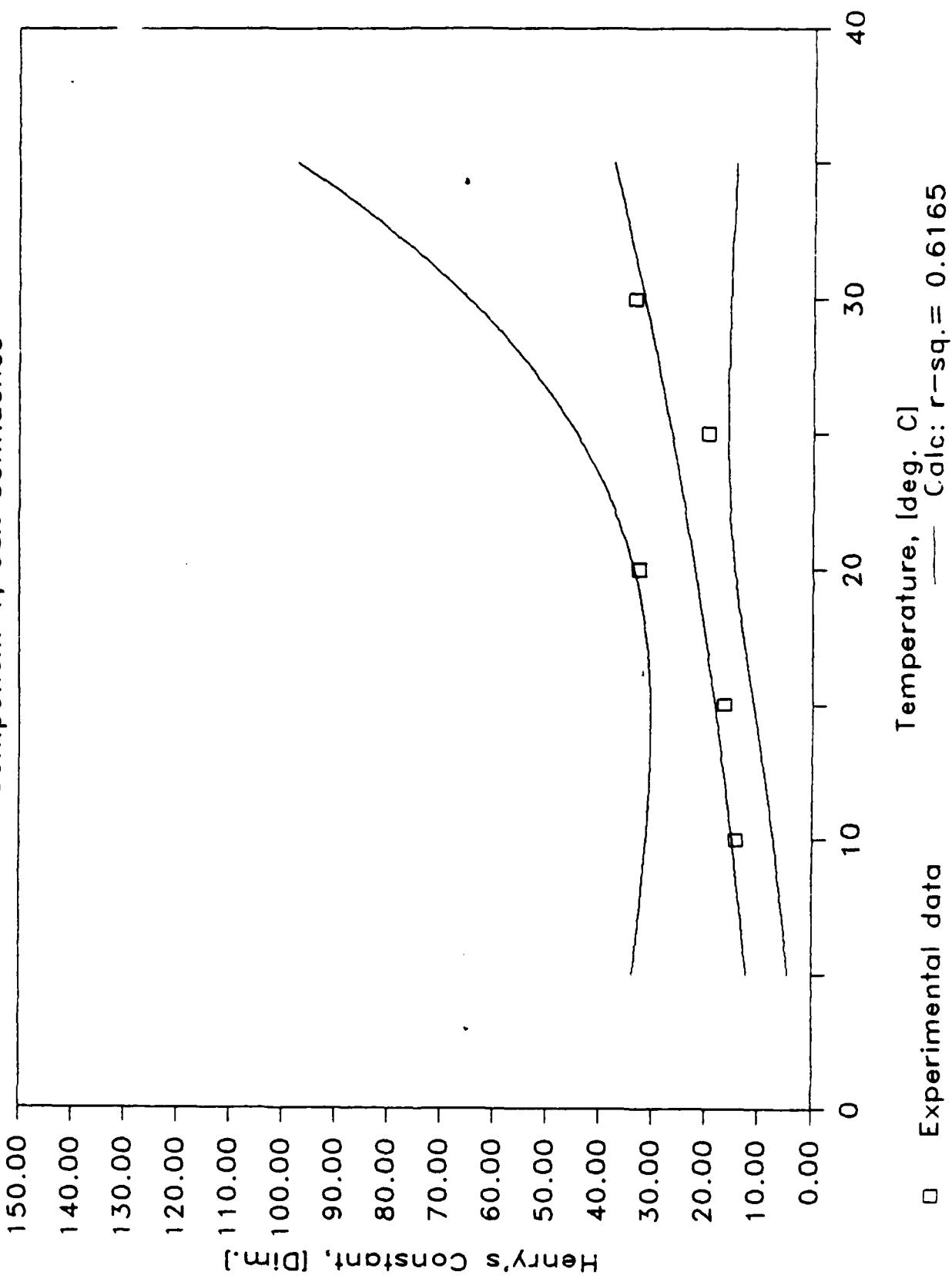
95% CONFIDENCE TEST

Component 1



REGRESSION CONFIDENCE TEST

Component 1, 95% Confidence



04-Nov-86

Results Summary for Component 101

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
REPLICATE -->	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	13		13		13	
Component ID	101		101		101	
Temperature (C)	11.3		15.15		20	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	17.1448	1.0E-25	20.9724	1.0E-25	13.7837	1.0E-25
H, avg: atm-mol/mol	22213.2		27540.1		18404.8	
H, avg: atm-m3/mol	4.00E-01	1	4.96E-01	1	3.32E-01	1
H, avg: kPa-m3/mol	40.5496		50.2737		33.5974	
COV, r [std/mean]	3.99		14.85		18.03	
COV, both replic.	_____		_____		_____	
Observation: (1)	16.6653		23.2082		11.0441	
[atm-m3/mol] (2)	17.8432		24.0825		13.5873	
(3)	16.4595		18.0233		13.4236	
(4)	17.6113		18.5757		17.0799	
Injection: (1)	159440		190570		164890	
[Peak Area] (2)	158980		181270		174500	
(3)	37812		42239		43692	
(4)	37234		41965		41151	

04-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	25	No. 1 No. 2	11	No. 1 No. 2
REPLICATE →				
Group No.	13		13	
Component ID	101		101	
Temperature (C)	25		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H, avg: atm=m3/mol	16.9283	1.0E-25	18.6762	1.0E-25
H, avg: atm=mol/mol	22989.0		25788.1	
H, avg: atm=m3/mol	4.14E-01	1	4.65E-01	1
H, avg: kPa=m3/mol	41.9658		47.0755	
COV, r [std/mean]	26.69		29.63	
COV, both replic.	_____		_____	
Observation: (1)	12.3382		18.2460	
[atm=m3/m3] (2)	18.0733		26.2694	
(3)	14.5921		13.0505	
(4)	22.7094		17.1389	
Injection: (1)	178030		168660	
[Peak Area] (2)	186320		155340	
(3)	45638		39196	
(4)	41459		36604	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

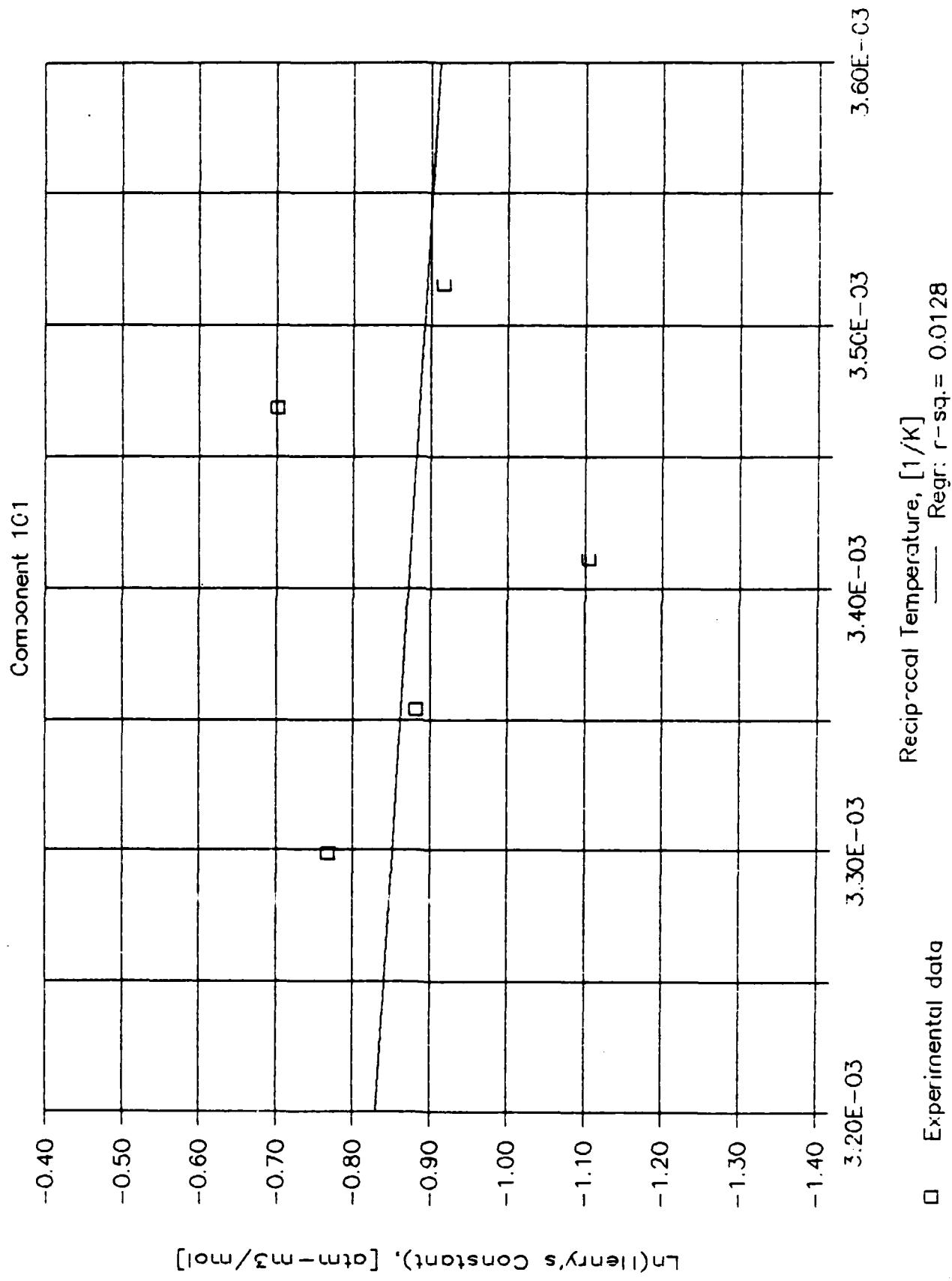
OF POINTS = 5

SLOPE = -2.0E+02

Y-INTERCEPT = -1.8E-01

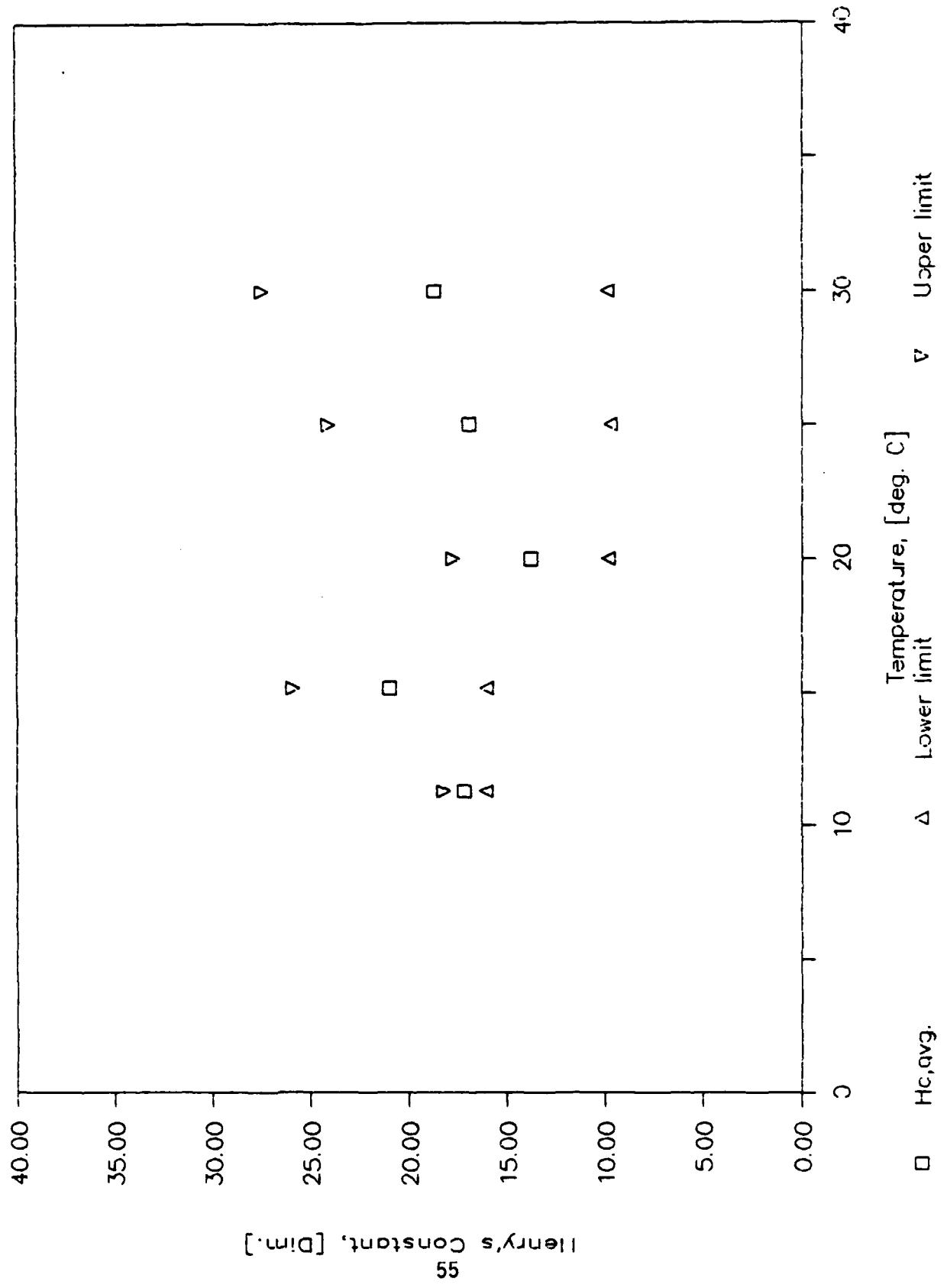
R-SQUARED = 0.0128

TEMPERATURE REGRESSION PLOT



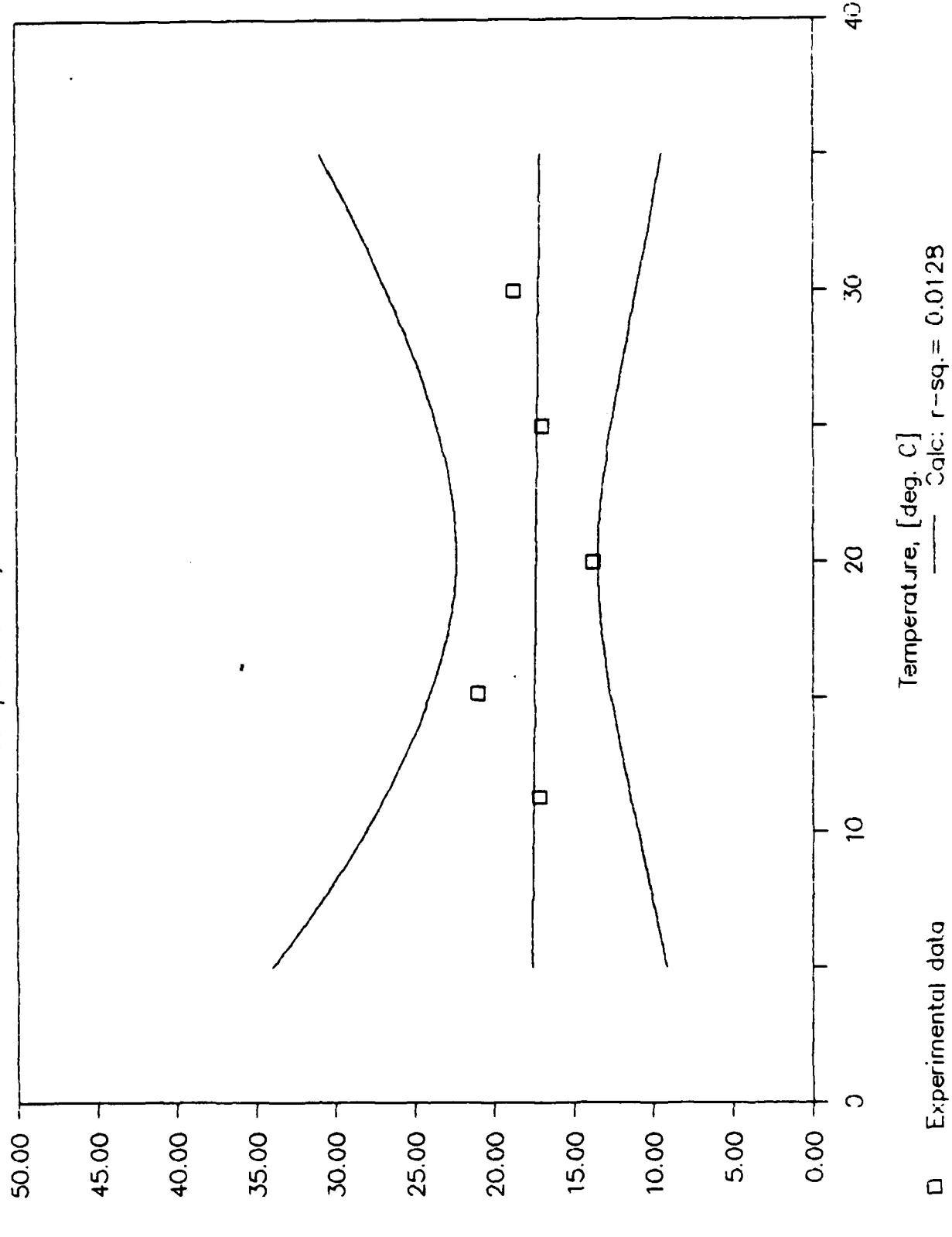
95% CONFIDENCE TEST

Component 1C1



REGRESSION CONFIDENCE TEST

Component 101, 95% Confidence



Henry's Constant [Dim.]

06-Nov-86

Results Summary for Component 2

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	6	6	6	6	7	7
REPLICATE →	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	1		1		1	
Component ID	2		2		2	
Temperature (C)	18		15		20	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H _v avg: atm-m ³ /mol	18.2642	1.0E-25	17.4885	1.0E-25	36.6895	1.0E-25
H _v avg: atm-mol/mol	13237.8		22953.3		48989.7	
H _v avg: atm-m ³ /mol	2.38E-01	1	4.14E-01	1	8.83E-01	1
H _v avg: kPa-m ³ /mol	24.1652		41.9886		89.4293	
COV, r [std/mean]	40.01		15.87		19.19	
COV, both replic.	_____		_____		_____	
Observation: (1)	6.7705		28.3232		41.3335	
(atm-m ³ /mol)	(2)	6.6504	19.3988		44.0424	
(3)	14.0131		15.4820		29.9597	
(4)	13.6229		14.8301		31.4223	
Injection: (1)	4239000		8138200		8947400	
[Peak Area]	(2)	5420000	7653500		8591000	
(3)	1341600		1849500		1827400	
(4)	1351700		1867000		1815100	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		7		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		1		1	
Component ID		2		2	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		31.3702	1.0E-25	62.7900	1.0E-25
H, avg: atm-mol/mol		42601.5		85700.4	
H, avg: atm-m3/mol		7.68E-01	1	1.56E+00	1
H, avg: kPa-m3/mol		77.7678		158.2698	
COV, r [std/mean]		16.61		31.65	
COV, both replic.		_____		_____	
Observations: (1)		25.7607		81.1600	
[atm-m3/mol] (2)		29.1638		78.7974	
(3)		32.5781		46.0037	
(4)		37.9781		45.1988	
Injections: (1)		6283300		4352700	
[Peak Area] (2)		6506900		4164900	
(3)		1368000		841100	
(4)		1341800		842670	

Temperature Regression Parameters:

OF POINTS = 5

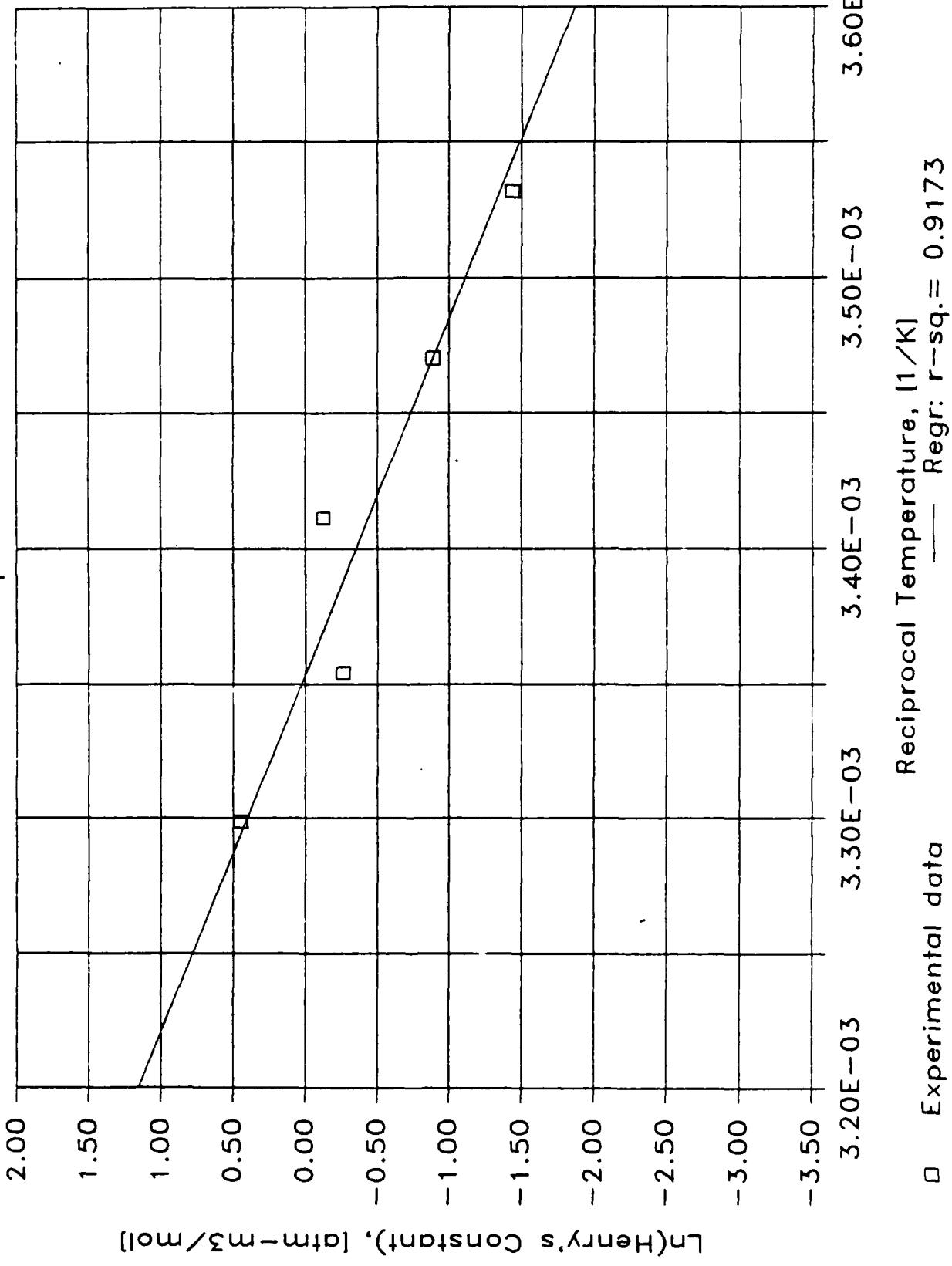
SLOPE = -7.5E+03

Y-INTERCEPT = 2.5E+01

R-SQUARED = 0.9173

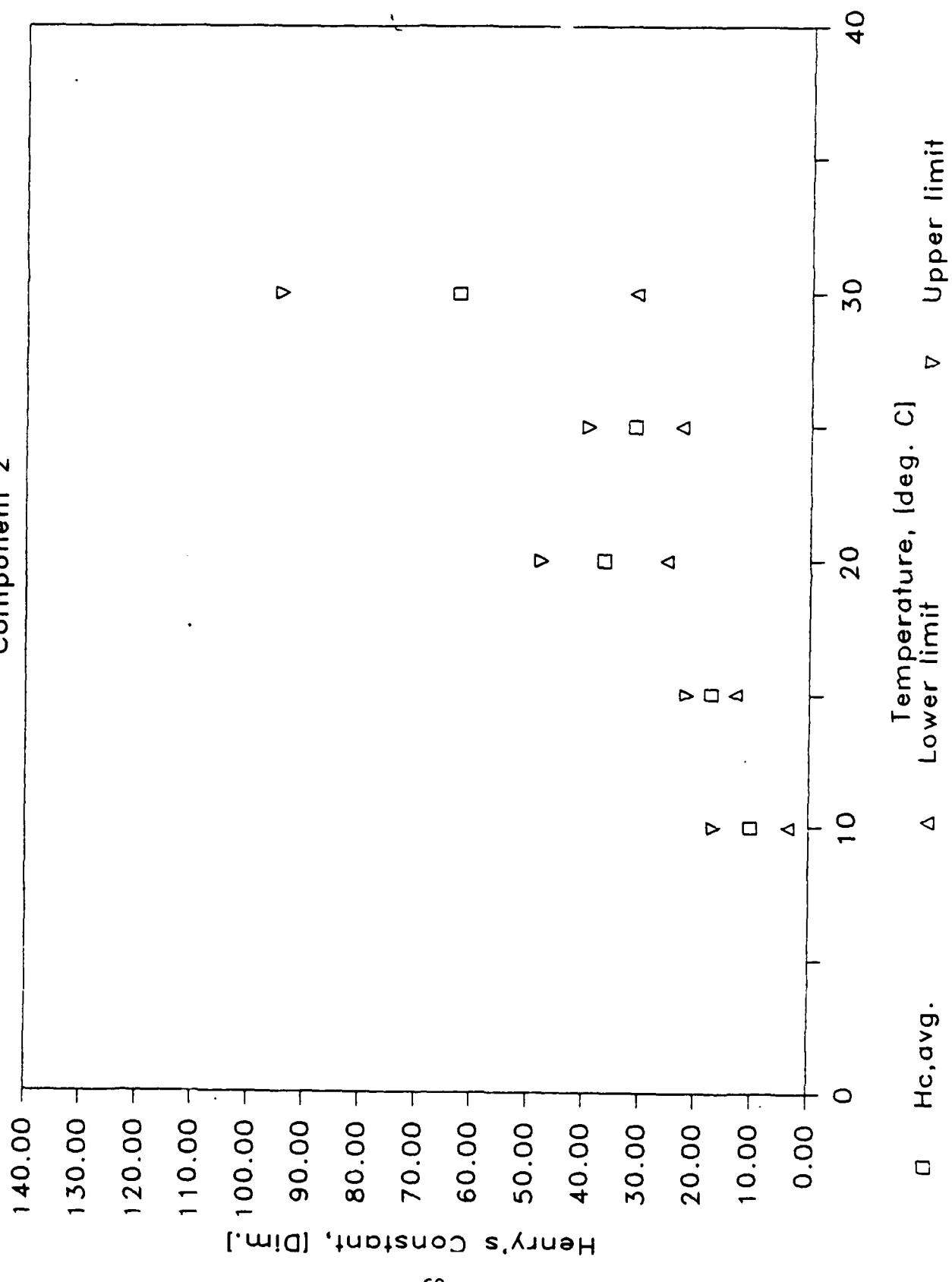
TEMPERATURE REGRESSION PLOT

Component 2



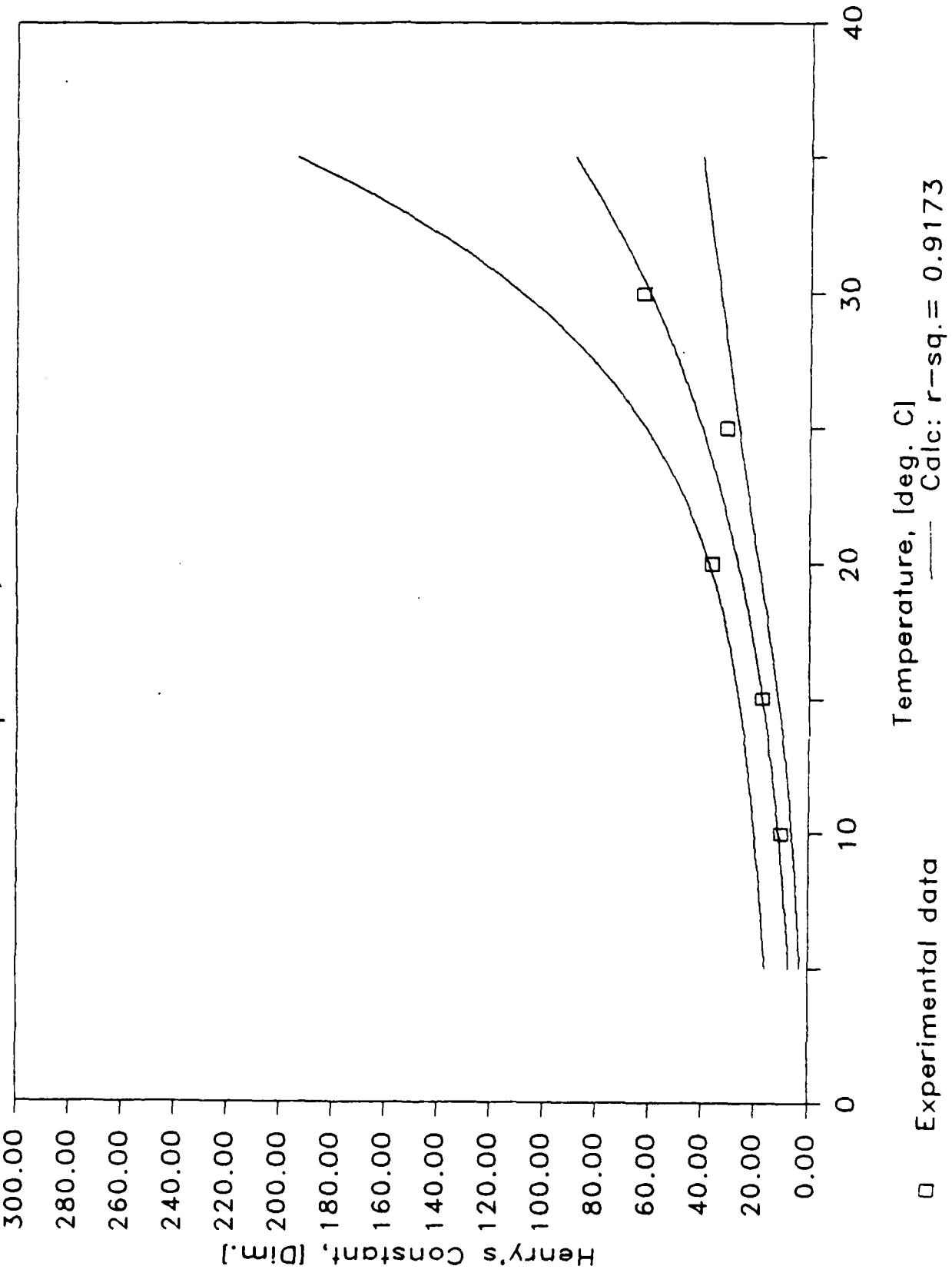
95% CONFIDENCE TEST

Component 2



REGRESSION CONFIDENCE TEST

Component 2, 95% Confidence



04-Nov-86

Results Summary for Component 102

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	6	No. 1	No. 2	20	No. 1	No. 2
REPLICATE -->						
Group No.		13		13		13
Component ID		102		102		102
Temperature (C)		11.3		15.15		20
Low Vol (ml)		30		30		30
High Vol (ml)		210		210		210
System Vol (ml)		250		250		250
H, avg: atm-m3/mol	28.5907	1.0E-25		19.4816	1.0E-25	-23.7783
H, avg: atm-mol/mol	37042.8			25582.4		-31750.0
H, avg: atm-m3/mol	6.67E-01	1		4.61E-01	1	***** 1
H, avg: kPa-m3/mol	67.6206			46.6999		-57.9587
COV, r [std/mean]	5.15			18.94		-191.62
COV, both replic.	_____			_____		_____
Observation: (1)	28.7444			16.2663		-66.3679
[atm-m3/mol] (2)	26.8502			16.3059		-59.9751
(3)	30.4330			22.6413		15.3265
(4)	28.3353			22.7126		15.9034
Injection: (1)	1456000			124620		89349
[Peak Area] (2)	1468200			133500		61960
(3)	311600			29722		14991
(4)	314890			29705		14857

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		21		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		13		13	
Component ID		102		102	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm=m3/mol		44.4458	1.0E-25	424.0461	1.0E-25
H, avg: atm=mol/mol		60358.5		585522.8	
H, avg: atm=m3/mol		1.09E+00	1	1.05E+01	1
H, avg: kPa=m3/mol		110.1827		*****	
COV, r [std/mean]		56.91		189.03	
COV, both replic.		_____		_____	
Observation: (1)		36.7509		-28.8881	
[atm=m3/mol] (2)		81.1478		*****	
(3)		23.1345		-34.1606	
(4)		36.7500		138.8790	
Injection: (1)		150070		1704900	
[Peak Area] (2)		140090		1649600	
(3)		31068		254850	
(4)		29002		310960	

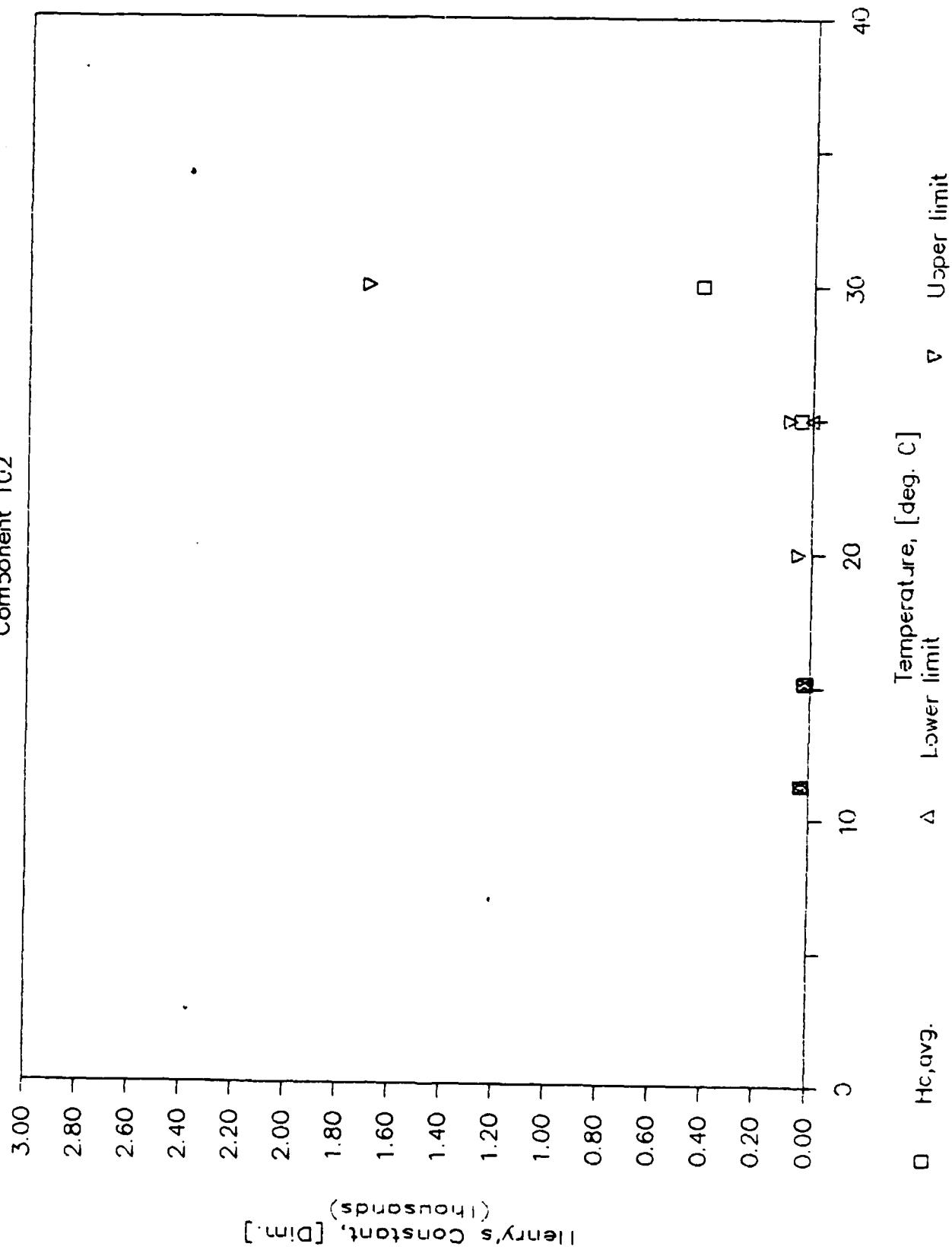
ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5
 SLOPE = ERR
 Y-INTERCEPT = ERR
 R-SQUARED = ERR

95% CONFIDENCE TEST

Component 1c2



(Thousands) [Dim.]

86-Nov-86

Results Summary for Component 3

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		10		10		11	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		1		1		1	
Component ID		3		3		3	
Temperature (C)		10		15		20	
Low Vol (ml)		30		30		30	
High Vol (ml)		210		210		210	
System Vol (ml)		250		250		250	
H ₂ avg: atm-m3/m3		38.0178	1.0E-25	29.3345	1.0E-25	26.2950	1.0E-25
H ₂ avg: atm-mol/mol		38714.0		38500.9		35110.4	
H ₂ avg: atm-m3/mol		6.97E-01	1	6.94E-01	1	6.33E-01	1
H ₂ avg: kPa-m3/mol		70.6713		70.2823		64.0931	
COV, r [std/mean]		23.49		15.31		18.00	
COV, both replic.		—	—	—	—	—	—
Observation: (1)		38.6247		27.2843		28.4660	
[atm-m3/m3] (2)		39.3879		24.5198		31.8405	
(3)		22.6544		34.8868		21.4523	
(4)		27.4040		30.7288		23.4212	
Injection: (1)		3382300		6615100		6471500	
[Peak Area] (2)		3145500		6851900		6167600	
(3)		700230		1427700		1387000	
(4)		678100		1452200		1364800	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		11		11	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		1		1	
Component ID		3		3	
Temperature (C)		25		39	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H _a avg: atm-m ³ /m ³		33.7896	1.0E-25	34.1064	1.0E-25
H _a avg: atm-mol/mol		45778.5		47894.8	
H _a avg: atm-m ³ /mol		8.25E-01	1	8.48E-01	1
H _a avg: kPa-m ³ /mol		83.5673		85.9688	
COV, r [std/mean]		16.31		79.75	
COV, both replic.		—		—	
Observation: (1)		27.6591		11.0221	
[atm-m ³ /m ³] (2)		33.8584		12.1452	
(3)		32.3777		46.8858	
(4)		40.9432		66.3724	
Injection: (1)		3311500		738898	
[Peak Area] (2)		3387900		971820	
(3)		712860		195910	
(4)		692660		198280	

Temperature Regression Parameters:

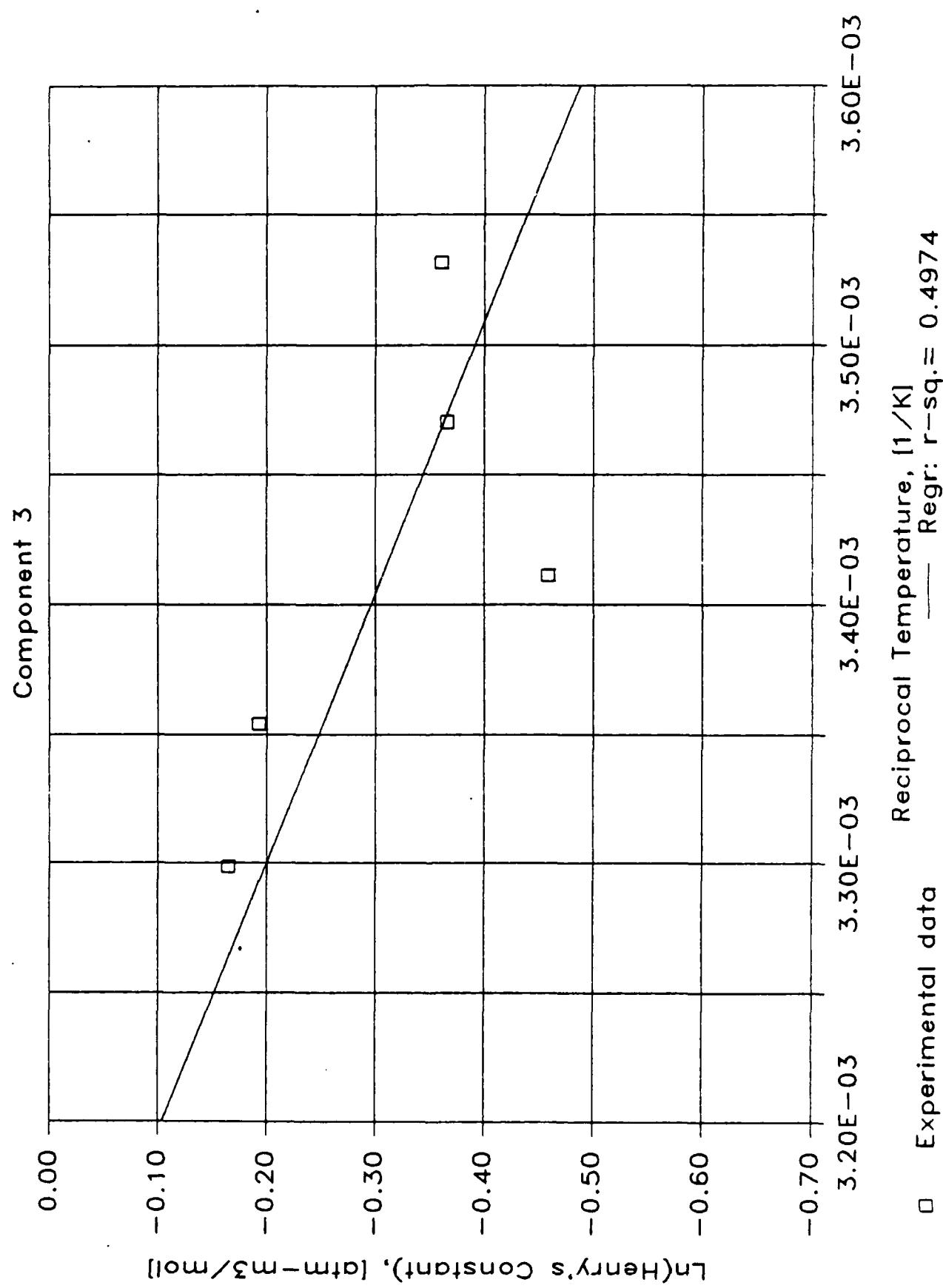
OF POINTS = 5

SLOPE = -9.6E+02

Y-INTERCEPT = 3.0E+00

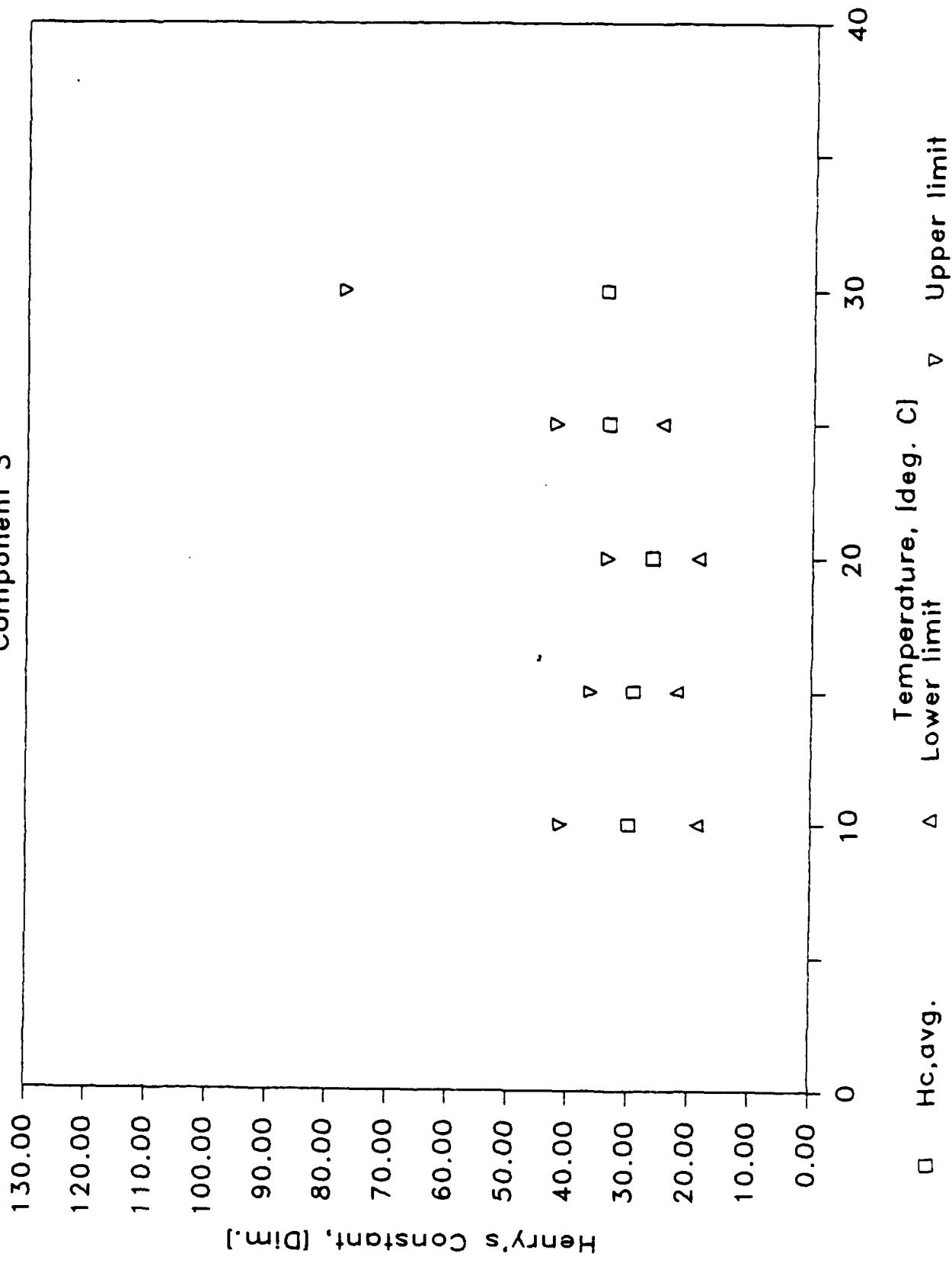
R-SQUARED = 0.4974

TEMPERATURE REGRESSION PLOT



95% CONFIDENCE TEST

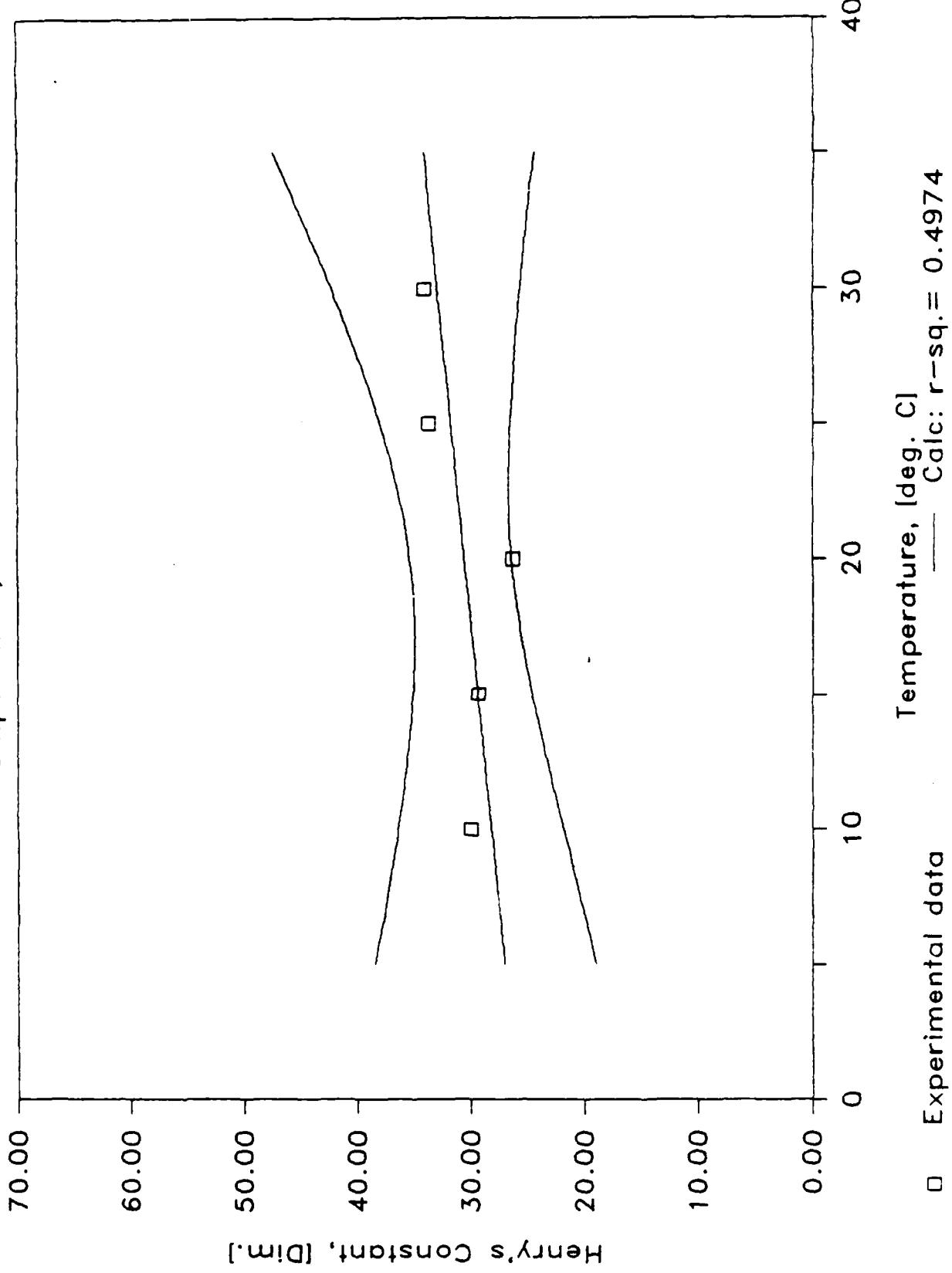
Component 3



Henry's Constant, (Dim.)

REGRESSION CONFIDENCE TEST

Component 3, 95% Confidence



04-Nov-86

Results Summary for Component 103

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	2	No. 1 No. 2	16	No. 1 No. 2	28	No. 1 No. 2
REPLICATE →						
Group No.		13		13		13
Component ID		103		103		103
Temperature (C)		11.3		15.2		20
Low Vol (ml)		30		30		30
High Vol (ml)		210		210		210
System Vol (ml)		250		250		250
H, avg: atm-m3/mol	35.1714	1.0E-25		8.6027	1.0E-25	8.4262
H, avg: atm-mol/mol	45569.0			11298.6		11251.1
H, avg: atm-m3/mol	8.21E-01	1		2.04E-01	1	2.03E-01
H, avg: kPa-m3/mol	83.1849			20.6253		20.5385
COV, r [std/mean]	18.99			19.10		69.26
COV, both replic.	—	—	—	—	—	—
Observation: (1)	30.1287			6.9932		3.3611
[atm-m3/mol] (2)	28.8115			9.6229		13.3835
(3)	42.0842			7.4320		3.3839
(4)	39.6614			10.3624		13.5762
Injection: (1)	431390			13660		7231
[Peak Area] (2)	449800			13999		7259
(3)	91687			4265		3237
(4)	92290			3785		1812

04-Nov-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	17	3	No. 1	No. 2
REPLICATE -->				
Group No.	13		13	
Component ID	103		103	
Temperature (C)	25		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H ₄ avg: atm=m3/m3	28.5047	1.0E-25	126.9938	1.0E-25
H ₄ avg: atm=mol/mol	38710.1		175353.1	
H ₄ avg: atm=m3/mol	6.97E-01	1	3.16E+00	1
H ₄ avg: kPa=m3/mol	70.6641		320.1020	
COV, r [std/mean]	88.64		66.41	
COV, both replic.	_____		_____	
Observation: (1)	8.0451		57.0423	
[atm=m3/m3] (2)	58.8220		69.2788	
(3)	7.3113		140.9994	
(4)	39.8402		240.6549	
Injection: (1)	15173		479350	
[Peak Area] (2)	14619		503960	
(3)	4483		94949	
(4)	2998		93575	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

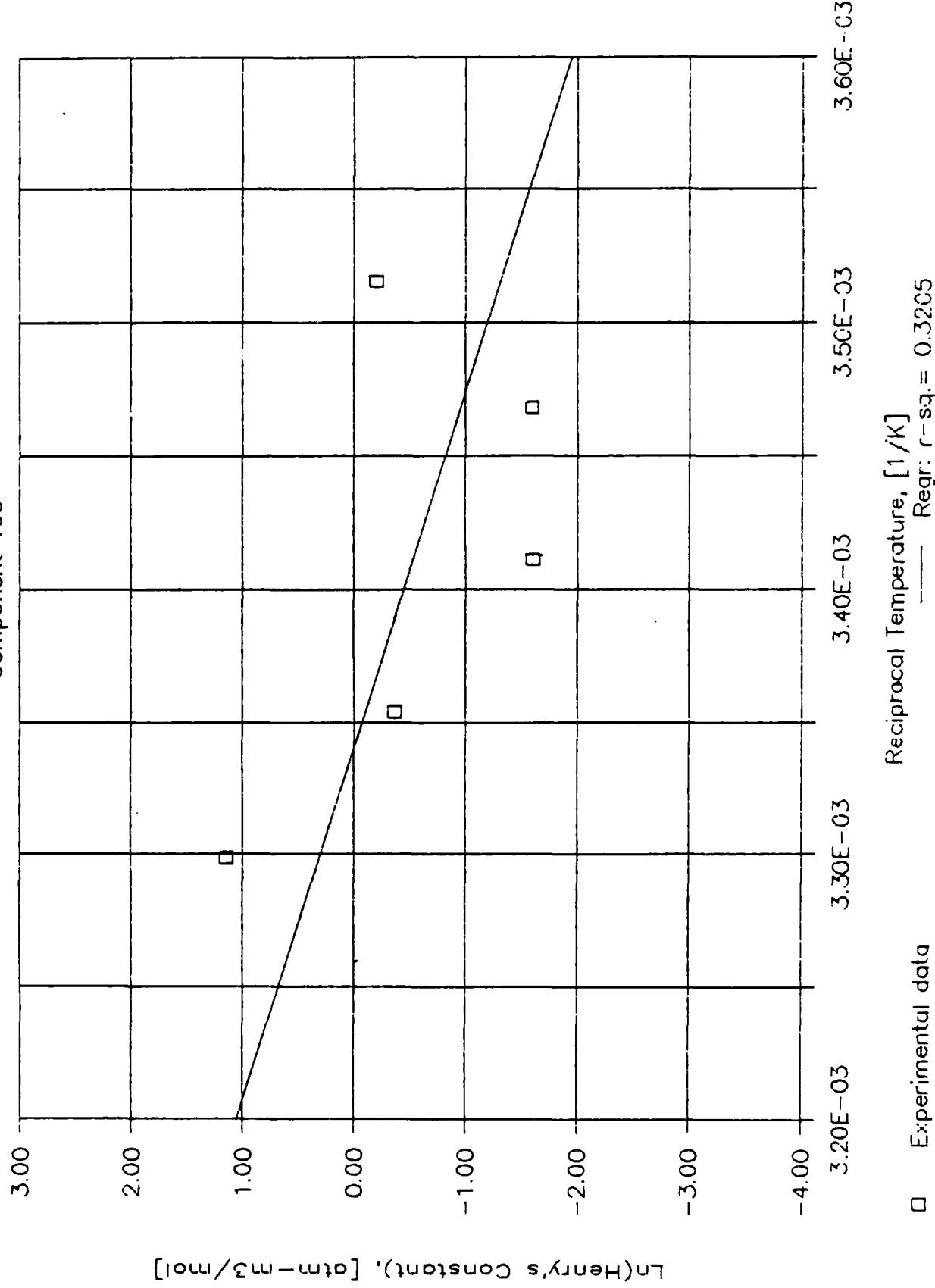
SLOPE = -7.5E+03

Y-INTERCEPT = 2.5E+01

R-SQUARED = 0.3205

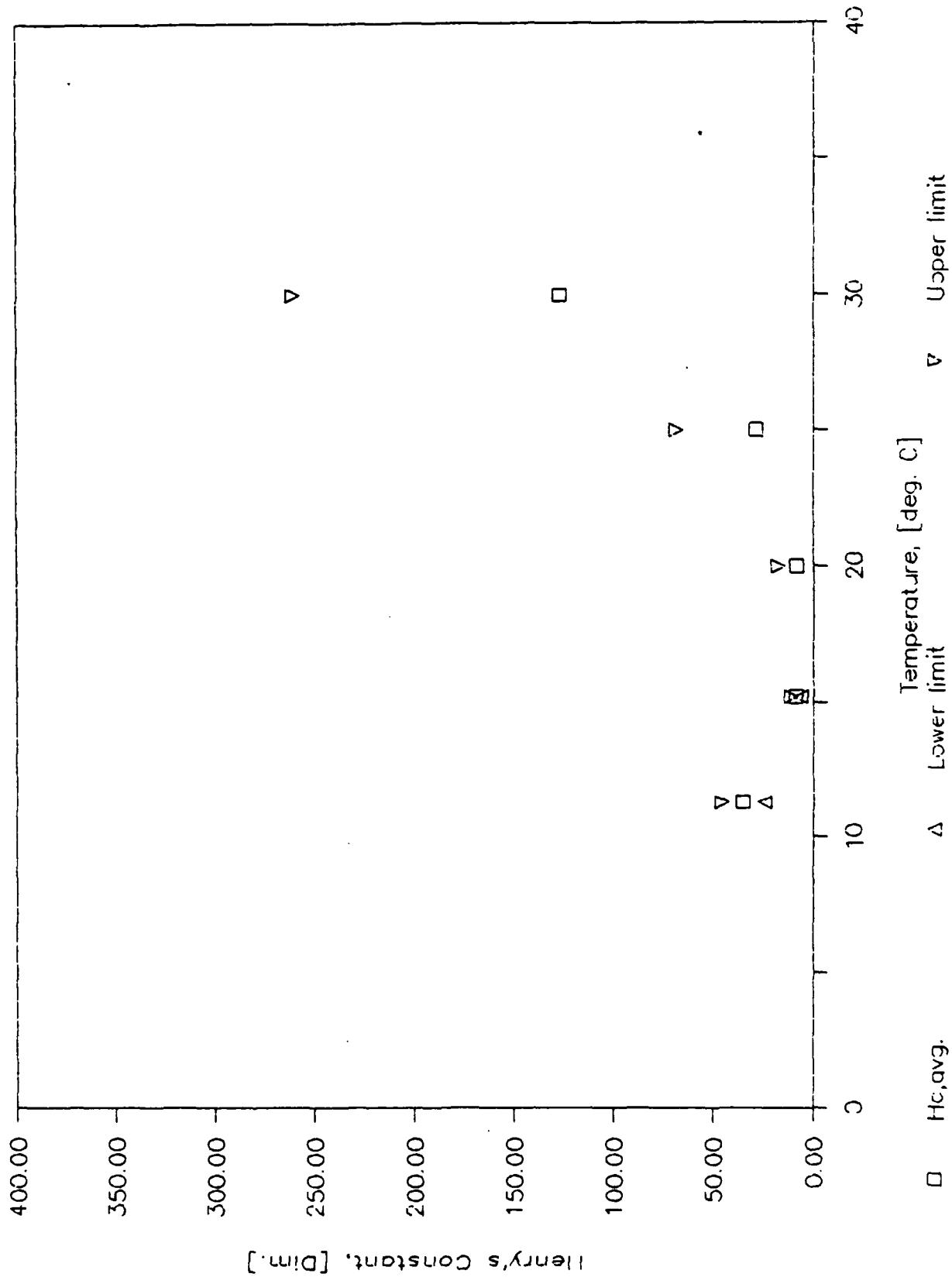
TEMPERATURE REGRESSION PLOT

Component 1C3



95% CONFIDENCE TEST

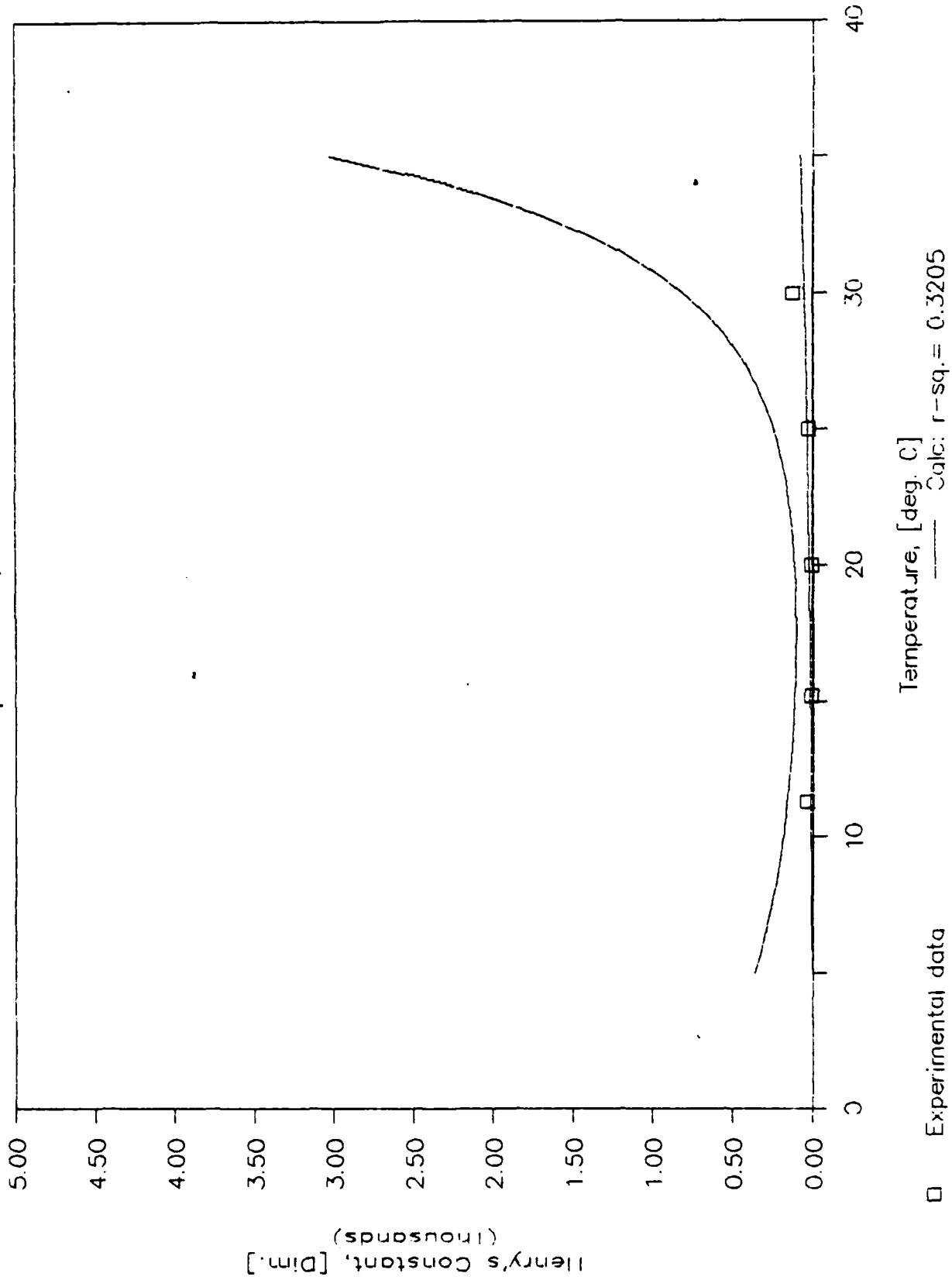
Component 1C3



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 103, 95% Confidence



06-Nov-86

Results Summary for Component 4

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	13	No. 1	No. 2	14	No. 1	No. 2
REPLICATE -->						
Group No.		1		1		1
Component ID		4		4		4
Temperature (C)		18		15		20
Low Vol (ml)		30		30		30
High Vol (ml)		210		210		210
System Vol (ml)		250		250		250
H _c avg: atm-m ³ /m ³	4.4272	1.0E-25		5.3138	1.0E-25	5.8816
H _c avg: atm-mol/mol	5709.7			6974.2		7746.7
H _c avg: atm-m ³ /mol	1.03E-01	1		1.26E-01	1	1.40E-01
H _c avg: kPa-m ³ /mol	18.4229			12.7312		14.1413
COV, r [std/mean]	1.76			7.03		11.47
COV, both replic.	—			—		—
Observation: (1)	4.4321			5.1285		5.2134
[atm-m ³ /m ³] (2)	4.5233			5.7465		5.2374
(3)	4.3324			4.9016		6.3617
(4)	4.4287			5.4785		6.3941
Injection: (1)	1614400			1607500		1620700
[Peak Area] (2)	1595600			1572600		1773900
(3)	622080			576150		576340
(4)	615650			546330		575000

86-Nov-86

Results Summary (continued)

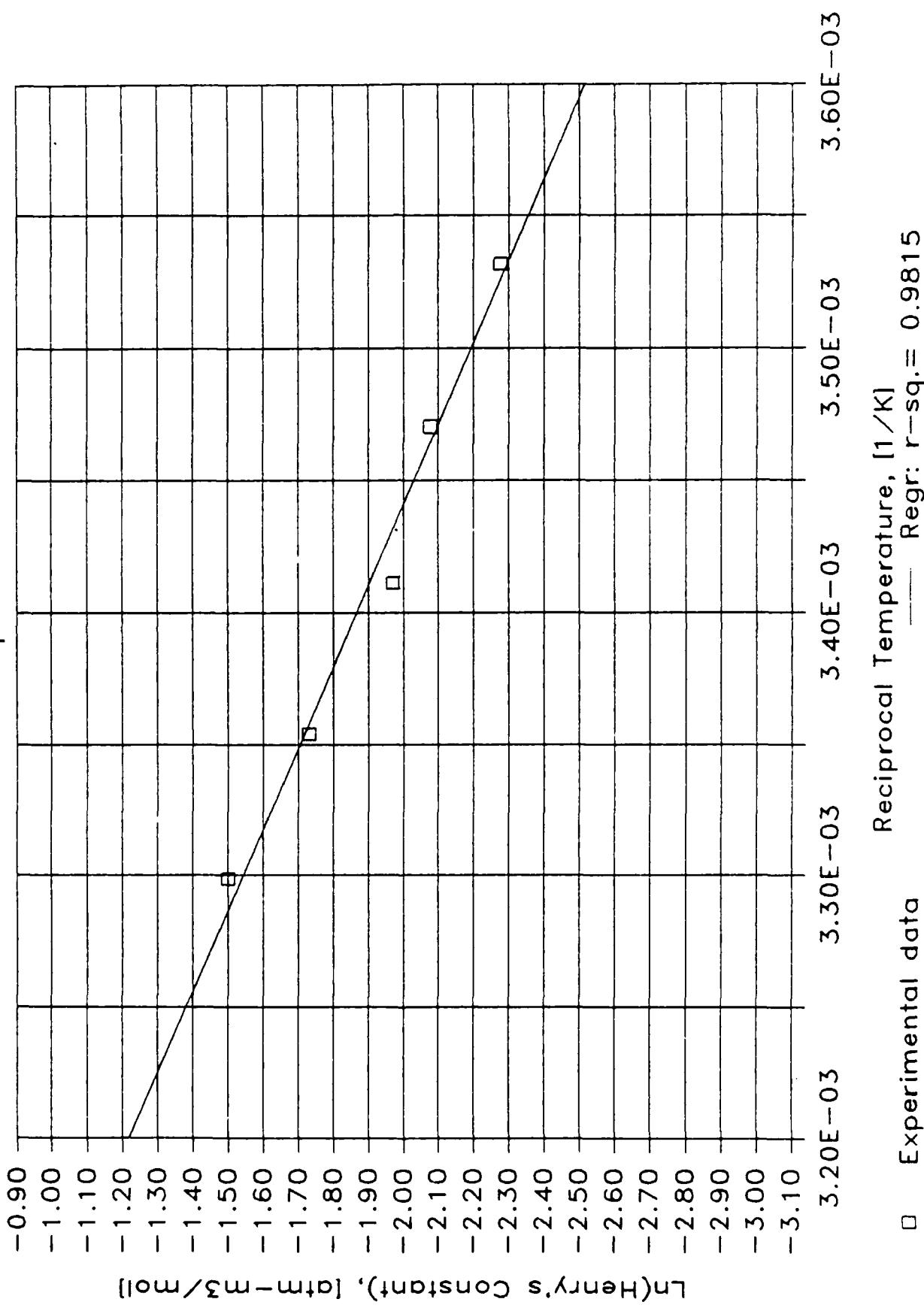
		Temperature 4		Temperature 5	
RUN Number -->		15		15	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		1		1	
Component ID		4		4	
Temperature (C)		25		38	
Low Vol (ml)		38		38	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H ₄ avg: atm-m ³ /m ³		7.2406	1.0E-25	8.9581	1.0E-25
H ₄ avg: atm-mol/mol		9832.9		12369.3	
H ₄ avg: atm-m ³ /mol		1.77E-01	1	2.23E-01	1
H ₄ avg: kPa-m ³ /mol		17.9496		22.5798	
COV, r [std/mean]		4.39		2.61	
COV, both replic.		—	—	—	—
Observation: (1)		7.4082		8.8352	
[atm-m ³ /m ³] (2)		7.5942		9.2280	
(3)		6.8968		8.7088	
(4)		7.0630		9.0761	
Injection: (1)		2064200		945450	
[Peak Area] (2)		2005300		940260	
(3)		629690		269880	
(4)		623570		265850	

Temperature Regression Parameters:

OF POINTS = 5
 SLOPE = -3.2E+03
 Y-INTERCEPT = 9.1E+00
 R-SQUARED = 0.9815

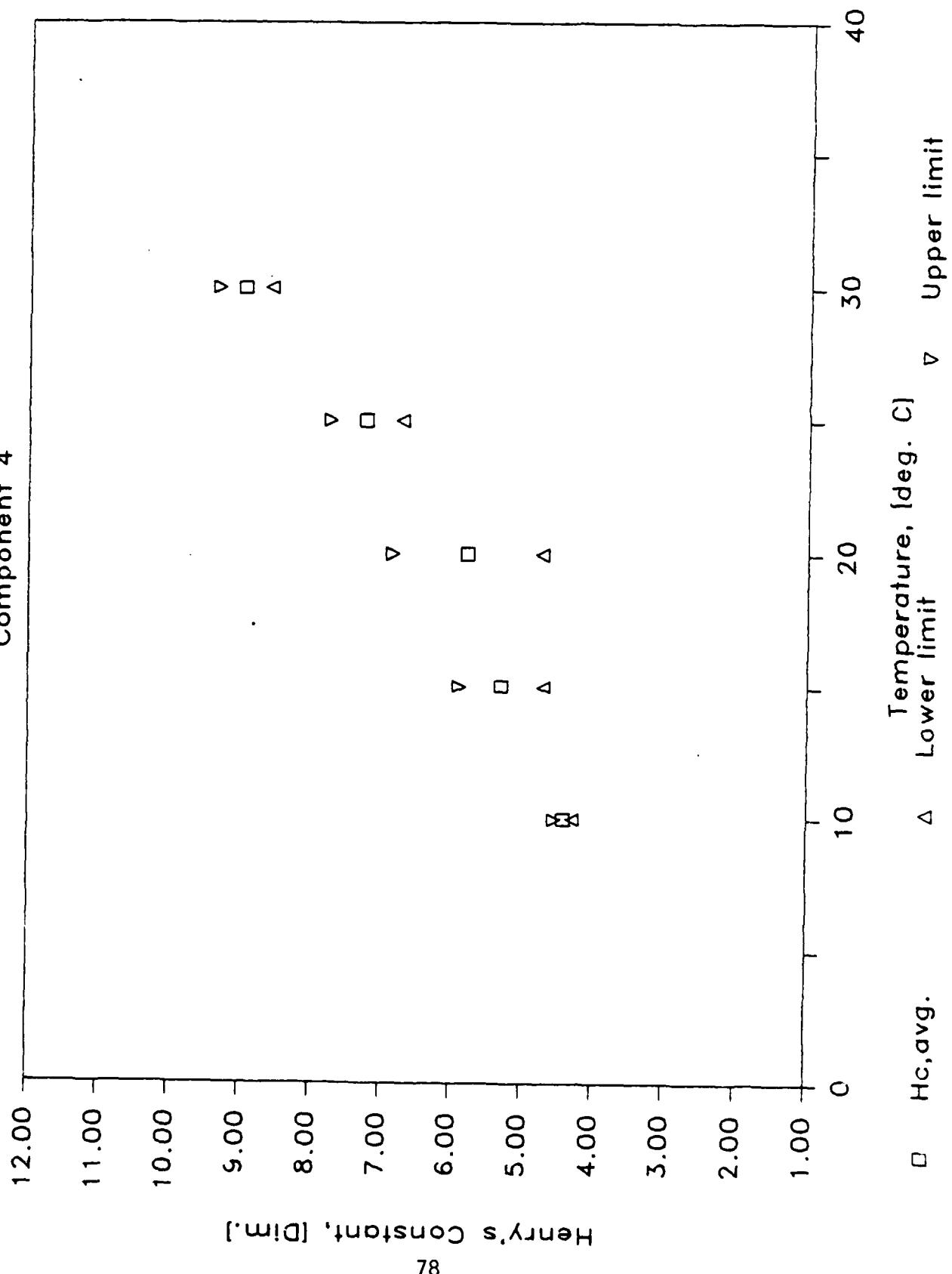
TEMPERATURE REGRESSION PLOT

Component 4



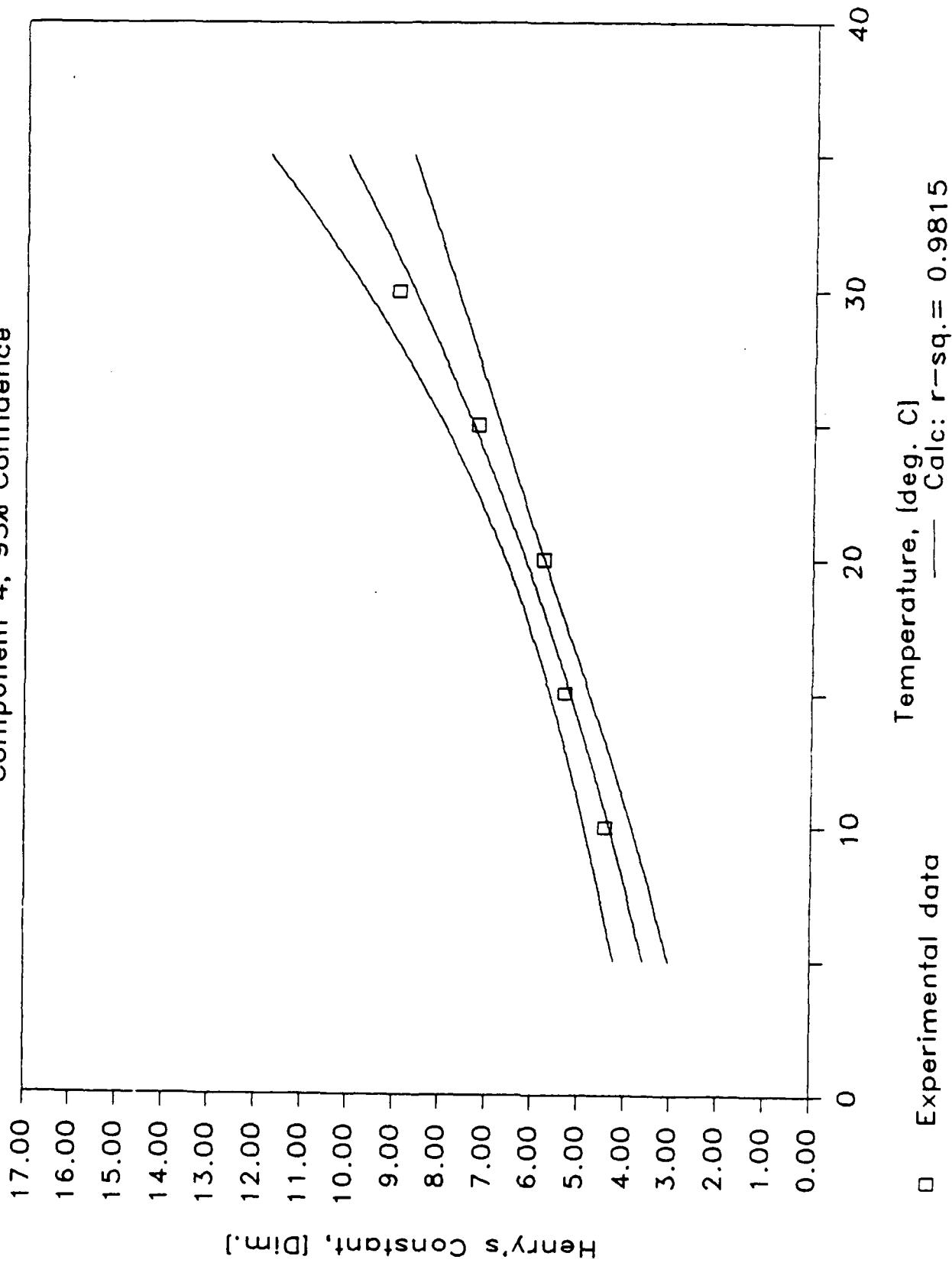
95% CONFIDENCE TEST

Component 4



REGRESSION CONFIDENCE TEST

Component 4, 95% Confidence



□ Experimental data

— Temperature, [deg. C]
Calc: $r^2 = 0.9815$

06-Nov-86

Results Summary for Component 5

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		2		3		4	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		2		2		2	
Component ID		5		5		5	
Temperature (C)		18		15		28.1	
Low Vol (ml)		25		25		25	
High Vol (ml)		285		285		285	
System Vol (ml)		250		250		250	
H _{avg} : atm-m ³ /m ³		0.0700	1.0E-25	0.0606	1.0E-25	0.0698	1.0E-25
H _{avg} : atm-mol/mol		90.3		79.6		93.3	
H _{avg} : atm-m ³ /mol		1.63E-03	1	1.43E-03	1	1.68E-03	1
H _{avg} : kPa-m ³ /mol		0.1648		0.1453		0.1703	
COV, r [std/mean]		12.19		7.63		4.29	
COV, both replic.		_____	_____	_____	_____	_____	_____
Observation: (1)		0.0748		0.0659		0.0739	
[atm-m ³ /m ³] (2)		0.0793		0.0585		0.0716	
(3)		0.0608		0.0628		0.0680	
(4)		0.0651		0.0554		0.0667	
Injection: (1)		392800		444368		534998	
[Peak Area] (2)		364460		436690		520980	
(3)		1956900		2319900		2689300	
(4)		1911800		2418000		2709200	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		3		1	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		2		2	
Component ID		5		5	
Temperature (C)		25		38	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H _v avg: atm-m3/m3		0.0641	1.0E-25	0.0953	1.0E-25
H _v avg: atm-mol/mol		87.1		131.6	
H _v avg: atm-m3/mol		1.57E-03	1	2.37E-03	1
H _v avg: kPa-m3/mol		0.1598		0.2482	
COV, r [std/mean]		8.56		10.56	
COV, both replic.		_____		_____	
Observation: (1)		0.0634		0.1028	
[atm-m3/m3] (2)		0.0575		0.0856	
(3)		0.0709		0.1051	
(4)		0.0647		0.0877	
Injection: (1)		600160		825380	
[Peak Area] (2)		633110		833670	
(3)		3218600		3594500	
(4)		3327500		3894300	

Temperature Regression Parameters:

OF POINTS = 5

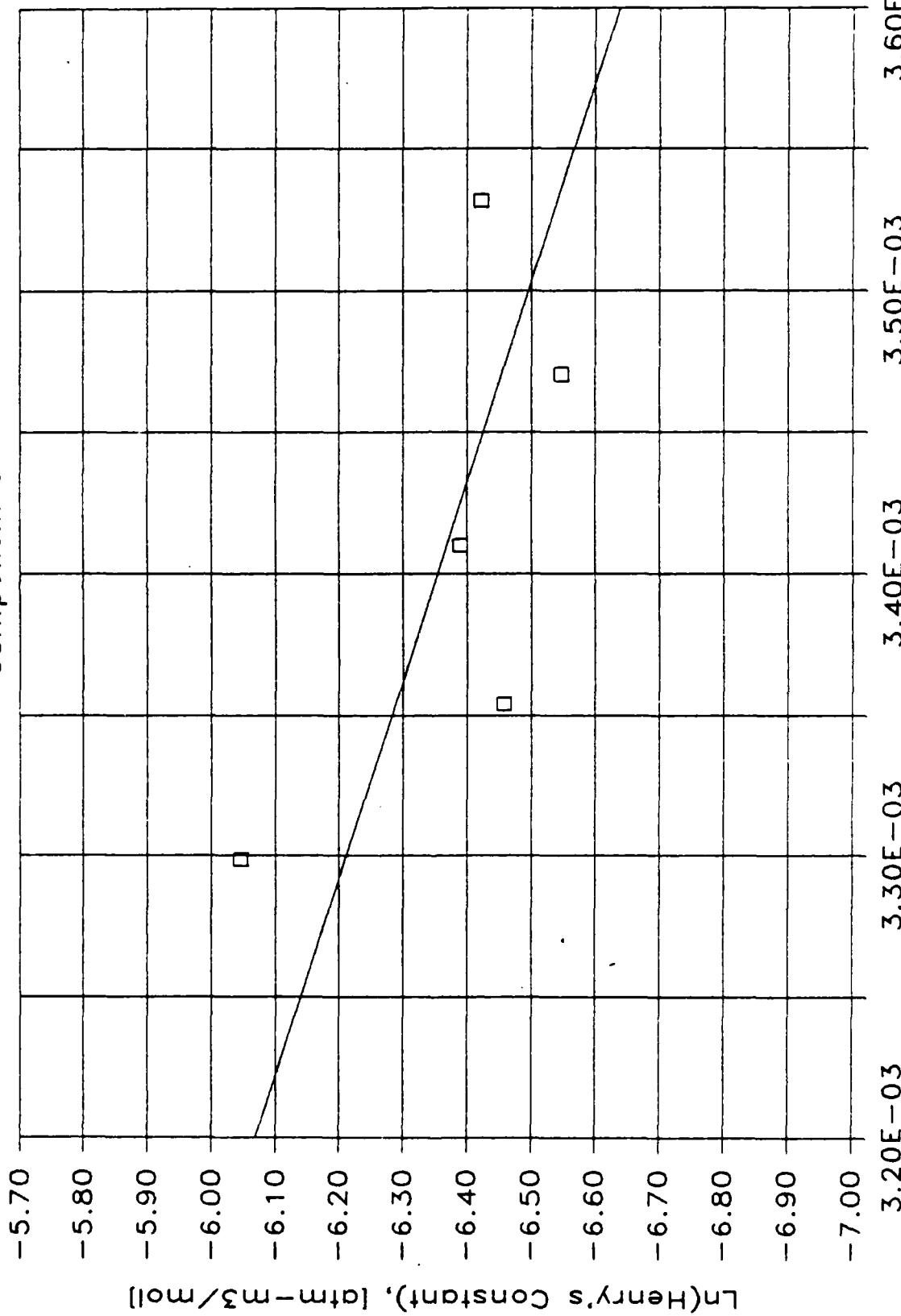
SLOPE = -1.4E+03

Y-INTERCEPT = -1.5E+00

R-SQUARED = 0.4641

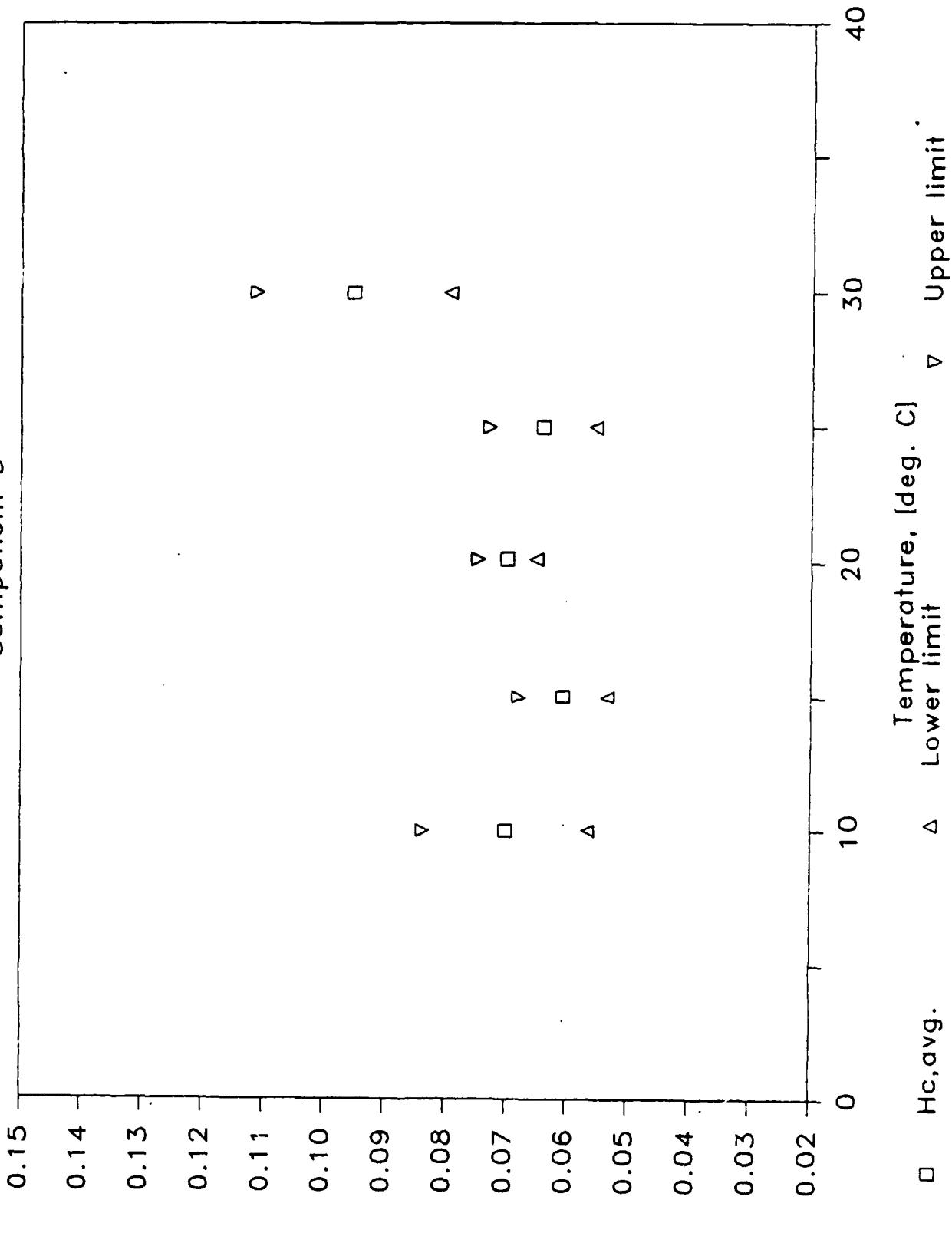
TEMPERATURE REGRESSION PLOT

Component 5



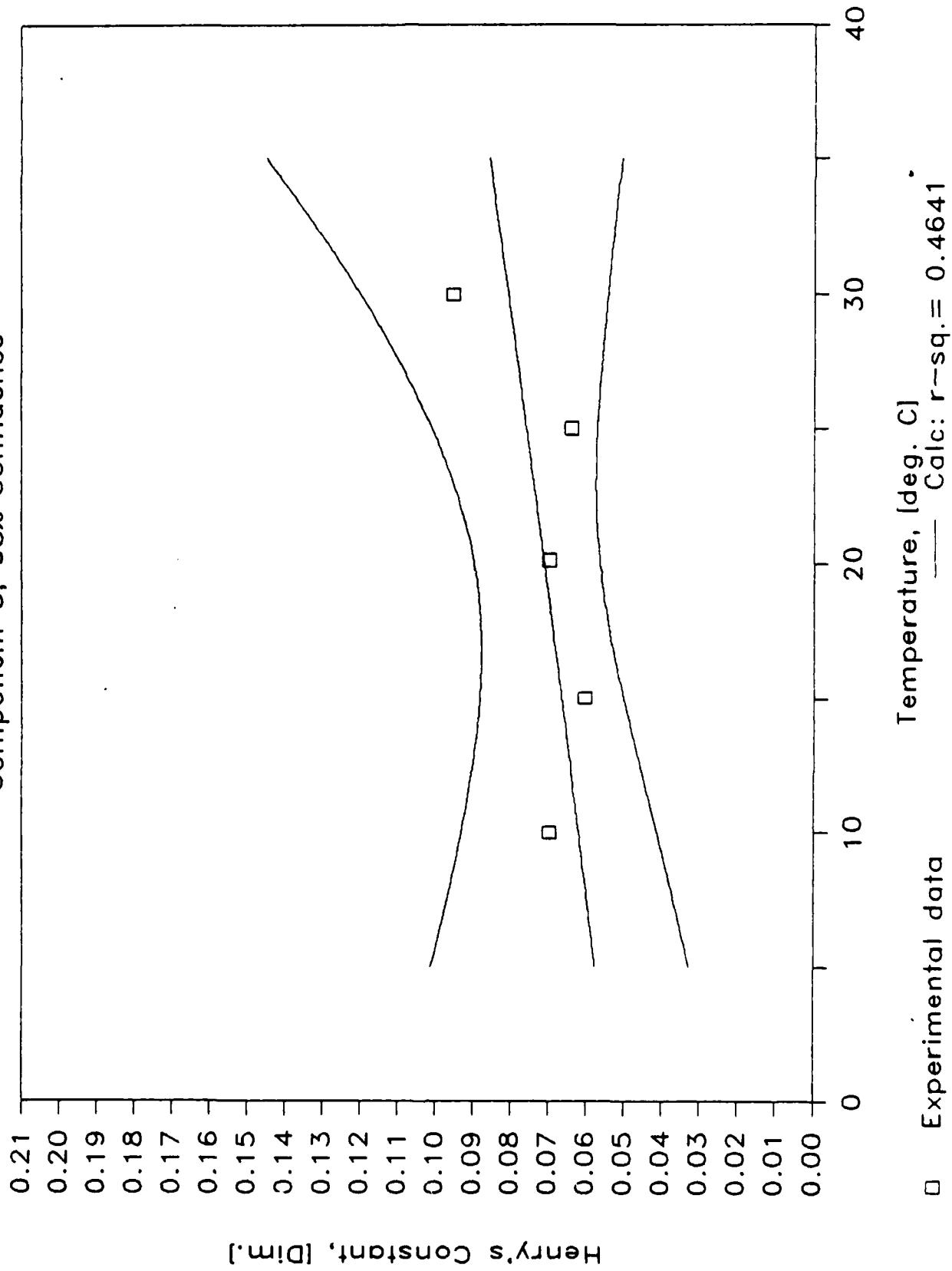
□ Experimental data — Reciprocal Temperature, [1/K]
□ Regr: r-sq. = 0.4641

95% CONFIDENCE TEST
Component 5



REGRESSION CONFIDENCE TEST

Component 5, 95% Confidence



Henry's Constant, [Dim.]

04-Nov-86

Results Summary for Component 105

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	75	No. 1 No. 2	87	No. 1 No. 2	100	No. 1 No. 2
REPLICATE →						
Group No.		14		14		14
Component ID		105		105		105
Temperature (C)		10.5		15.3		19.5
Low Vol (ml)		25		25		25
High Vol (ml)		205		205		205
System Vol (ml)		250		250		250
H ₄ avg: atm-m ³ /mol		0.0522 1.0E-25		0.0463 1.0E-25		0.0848 1.0E-25
H ₄ avg: atm-mol/mol		67.4		60.9		113.1
H ₄ avg: atm-m ³ /mol		1.21E-03 1		1.10E-03 1		2.04E-03 1
H ₄ avg: kPa-m ³ /mol		0.1231		0.1111		0.2065
COV, r [std/mean]		33.04		39.24		11.05
COV, both replic.		_____		_____		_____
Observation: (1)		0.0706		0.0631		0.0949
[atm-m ³ /mol]	(2)	0.0627		0.0610		0.0904
	(3)	0.0410		0.0314		0.0791
	(4)	0.0344		0.0298		0.0749
Injection:	(1)	284150		291240		327710
[Peak Area]	(2)	239340		240000		303580
	(3)	1446700		1544500		1479300
	(4)	1509700		1562100		1511100

04-Nov-86

Results Summary (continued)

RUN Number —>	Temperature 4		Temperature 5	
	88	76	No. 1	No. 2
REPLICATE —>				
Group No.	14		14	
Component ID	105		105	
Temperature (C)	25.2		30	
Low Vol (ml)	25		25	
High Vol (ml)	205		205	
System Vol (ml)	250		250	
H, avg: atm-m3/m3	0.0756	1.0E-25	0.1075	1.0E-25
H, avg: atm-mol/mol	102.7		148.4	
H, avg: atm-m3/mol	1.85E-03	1	2.67E-03	1
H, avg: kPa-m3/mol	0.1875		0.2709	
COV, r [std/mean]	11.32		4.12	
COV, both replic.	—		—	
Observation: (1)	0.0817		0.1113	
[atm-m3/m3] (2)	0.0841		0.1037	
(3)	0.0672		0.1113	
(4)	0.0694		0.1036	
Injection: (1)	457630		673370	
[Peak Area] (2)	424430		673320	
(3)	2200900		2825700	
(4)	2175200		2921700	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

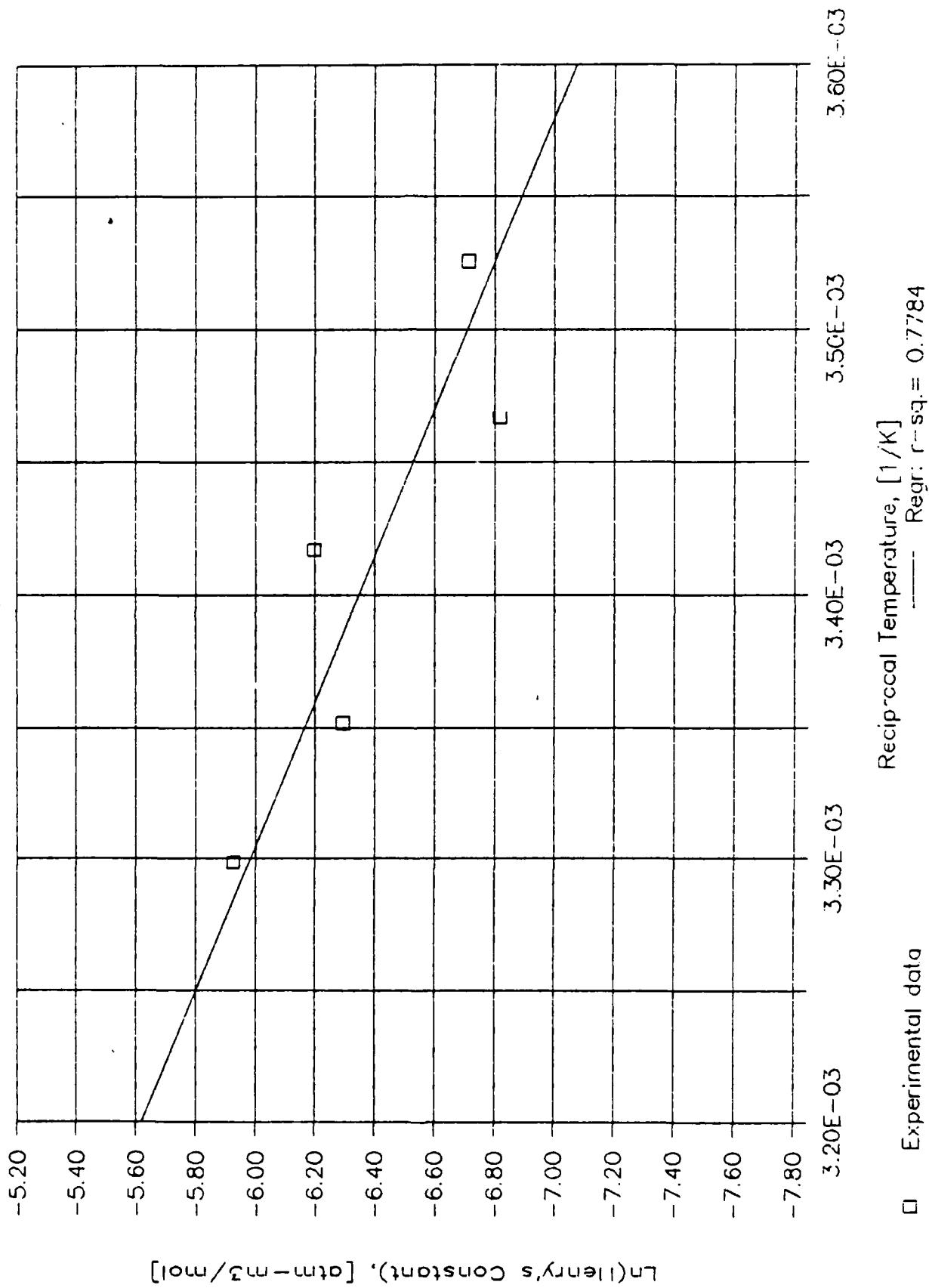
SLOPE = -3.6E+03

Y-INTERCEPT = 6.0E+00

R-SQUARED = 0.7784

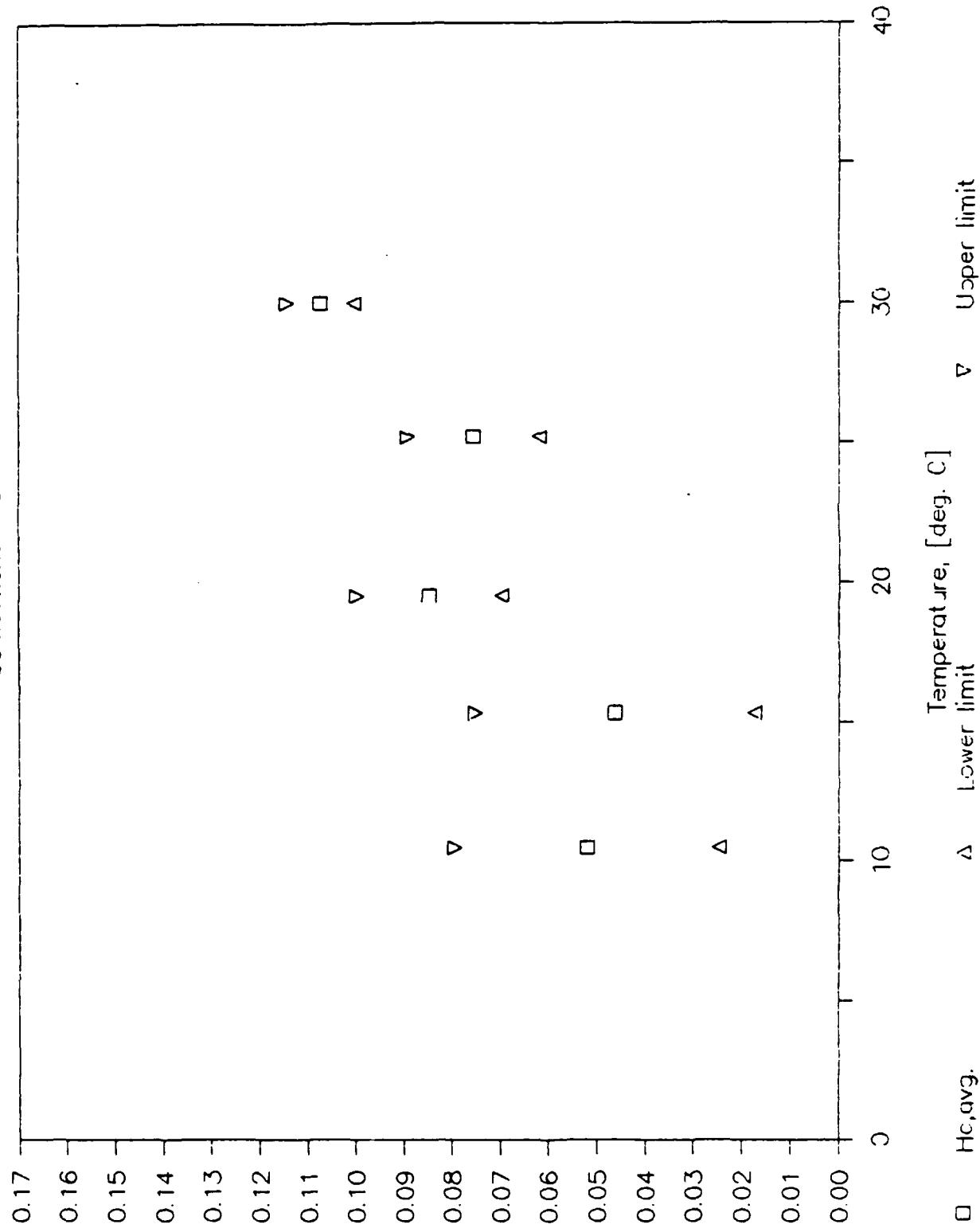
TEMPERATURE REGRESSION PLOT

Component 105



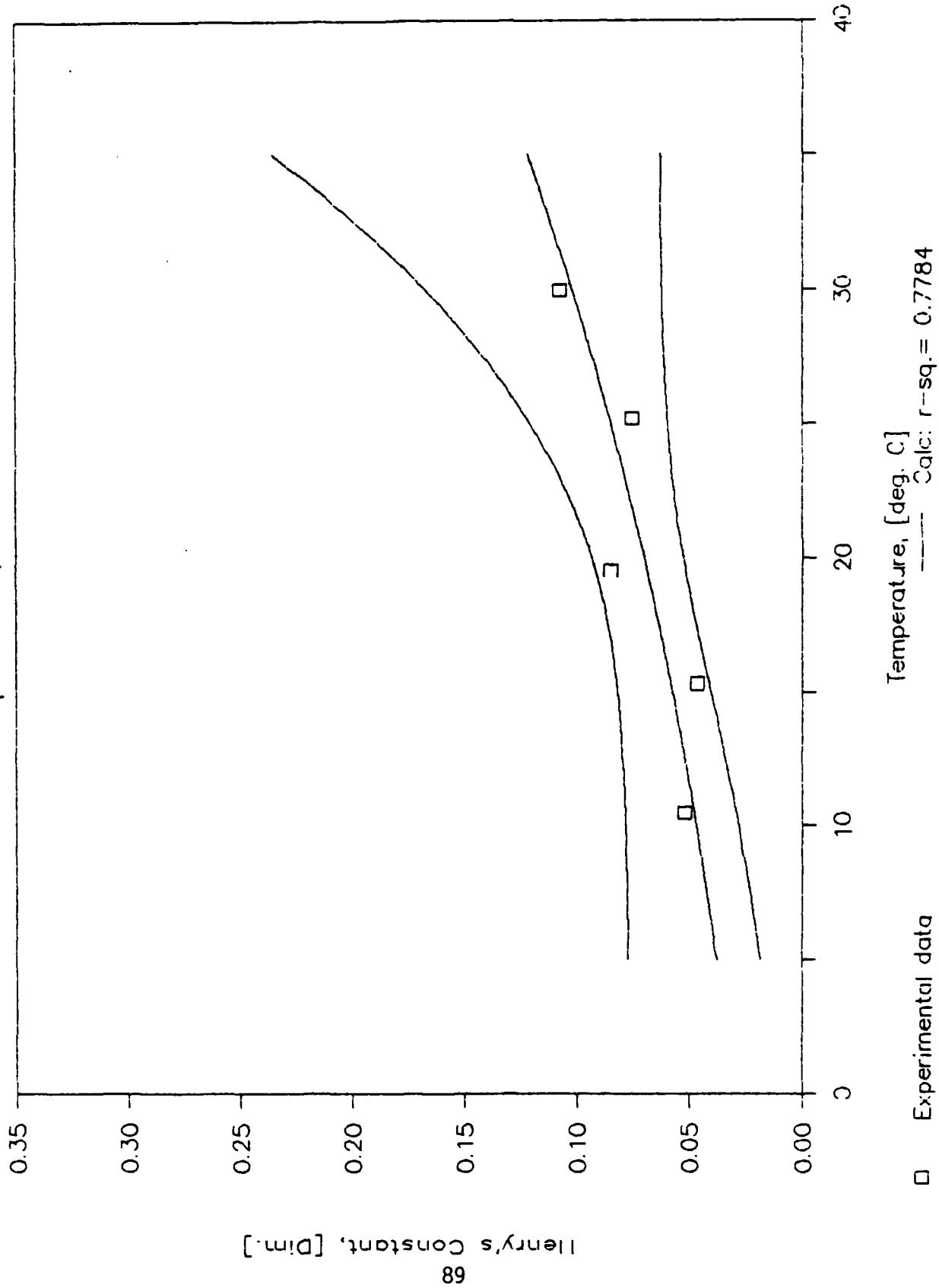
95% CONFIDENCE TEST

Component 1c5



REGRESSION CONFIDENCE TEST

Component 105, 95% Confidence



Henry's Constant, [Dim.]

06-Nov-86

Results Summary for Component 6

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	2		2		2	
Component ID	6		6		6	
Temperature (C)	10		15		20.1	
Low Vol (ml)	25		25		25	
High Vol (ml)	205		205		205	
System Vol (ml)	250		250		250	
H _c avg: atm-m ³ /m ³	0.1052	1.0E-25	0.1188	1.0E-25	0.1417	1.0E-25
H _c avg: atm-mol/mol	135.7		155.9		189.2	
H _c avg: atm-m ³ /mol	2.44E-03	1	2.81E-03	1	3.41E-03	1
H _c avg: kPa-m ³ /mol	0.2477		0.2846		0.3455	
COV, r [std/mean]	7.23		1.00		1.60	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.1079		0.1181		0.1401	
[atm-m ³ /m ³] (2)	0.1142		0.1200		0.1394	
(3)	0.0964		0.1173		0.1440	
(4)	0.1024		0.1195		0.1432	
Injection: (1)	332510		409510		486310	
[Peak Area] (2)	315850		408560		493360	
(3)	1416100		1670200		1817900	
(4)	1378400		1656600		1822900	

06-Nov-86

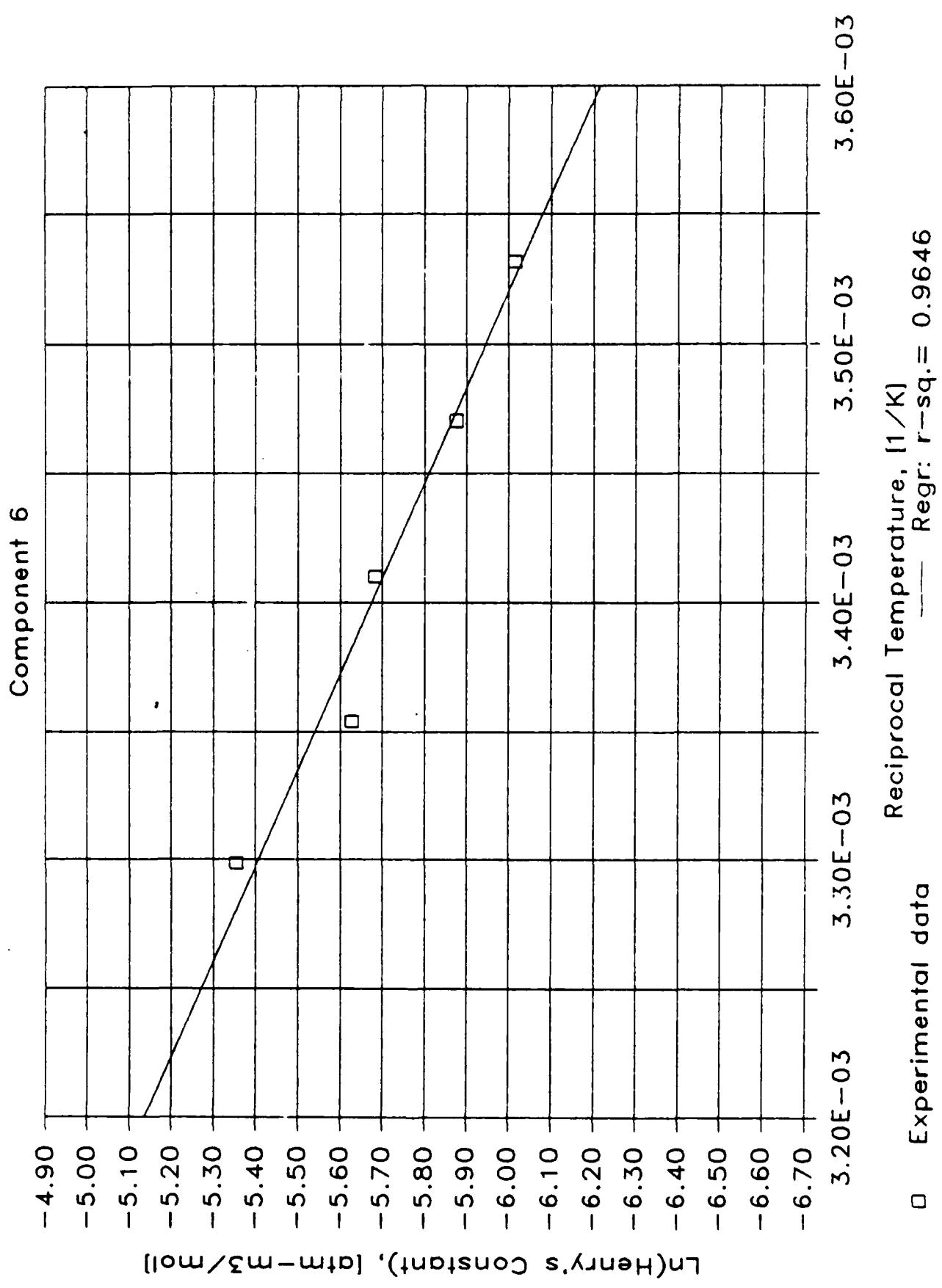
Results Summary (continued)

RUN Number —>	Temperature 4		Temperature 5	
	7	5	5	2
REPLICATE —>	No. 1	No. 2	No. 1	No. 2
Group No.	2		2	
Component ID	6		6	
Temperature (C)	25		30	
Low Vol (ml)	25		25	
High Vol (ml)	205		205	
System Vol (ml)	250		250	
H ₄ avg: atm-m ³ /mol	0.1470	1.0E-25	0.1902	1.0E-25
H ₄ avg: atm-mol/mol	199.7		262.7	
H ₄ avg: atm-m ³ /mol	3.60E-03	1	4.73E-03	1
H ₄ avg: kPa-m ³ /mol	0.3645		0.4795	
COV, r [std/mean]	0.76		0.97	
COV, both replic.	_____		_____	
Observation: (1)	0.1476		0.1892	
[atm-m ³ /mol]	(2)	0.1483	0.1922	
	(3)	0.1458	0.1883	
	(4)	0.1465	0.1913	
Injection: (1)	556060		727340	
[Peak Area]	(2)	552440	725320	
	(3)	2022100	2298600	
	(4)	2016400	2276900	

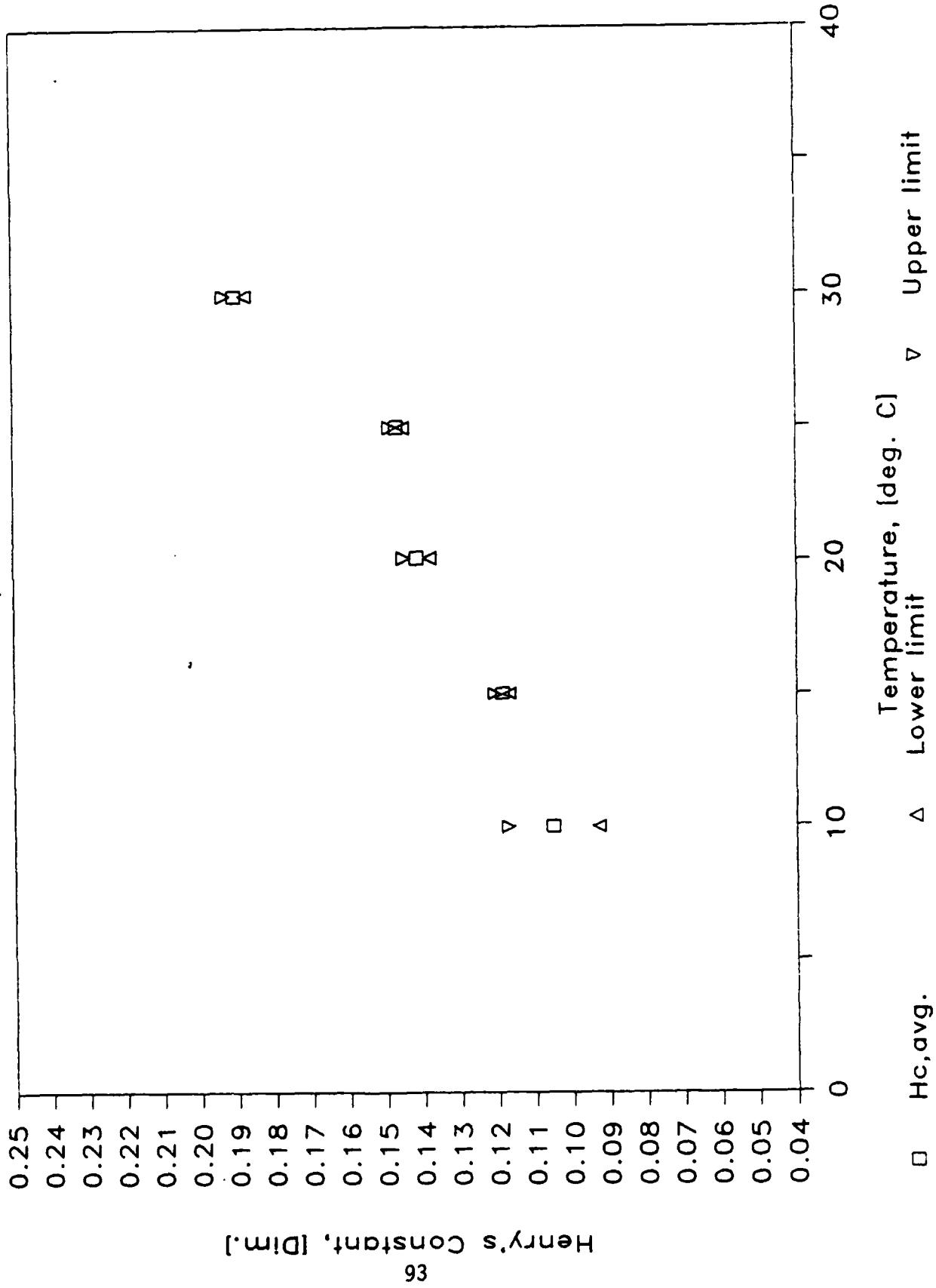
Temperature Regression Parameters:

OF POINTS = 5
 SLOPE = -2.7E+03
 Y-INTERCEPT = 3.5E+00
 R-SQUARED = 0.9646

TEMPERATURE REGRESSION PLOT

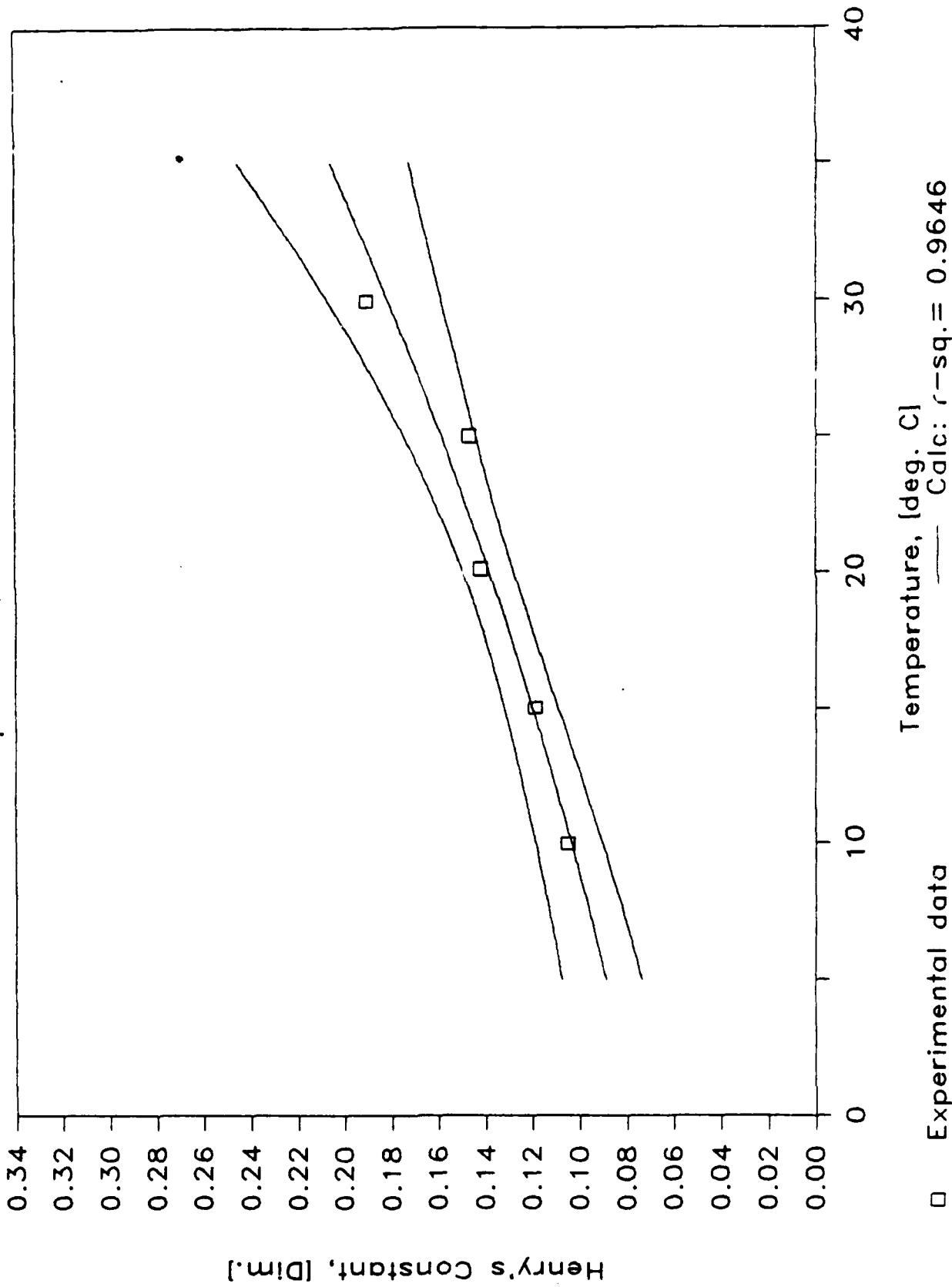


95% CONFIDENCE TEST
Component 6



REGRESSION CONFIDENCE TEST

Component 6, 95% Confidence



Henry's Constant, [Dim.]

86-Nov-86

Results Summary for Component 7

		Temperature 1		Temperature 2		Temperature 3	
RUN Number —>		10		11		12	
REPLICATE —>		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		2		2		2	
Component ID		7		7		7	
Temperature (C)		10		15		20.1	
Low Vol (ml)		25		25		25	
High Vol (ml)		285		285		285	
System Vol (ml)		250		250		250	
H ₄ avg: atm-m3/m3		0.0953	1.0E-25	0.0977	1.0E-25	0.1221	1.0E-25
H ₄ avg: atm-mol/mol		122.9		128.2		163.0	
H ₄ avg: atm-m3/mol		2.21E-03	1	2.31E-03	1	2.94E-03	1
H ₄ avg: kPa-m3/mol		0.2244		0.2341		0.2976	
COV, r [std/mean]		9.48		5.99		3.81	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.1063		0.1033		0.1215	
[atm-m3/m3] (2)		0.0971		0.1022		0.1278	
(3)		0.0932		0.0932		0.1164	
(4)		0.0946		0.0921		0.1225	
Injection: (1)		598440		553140		694170	
[Peak Area] (2)		471490		528210		679760	
(3)		2145900		2404100		2791500	
(4)		2236100		2415600		2721900	

06-Nov-86

Results Summary (continued)

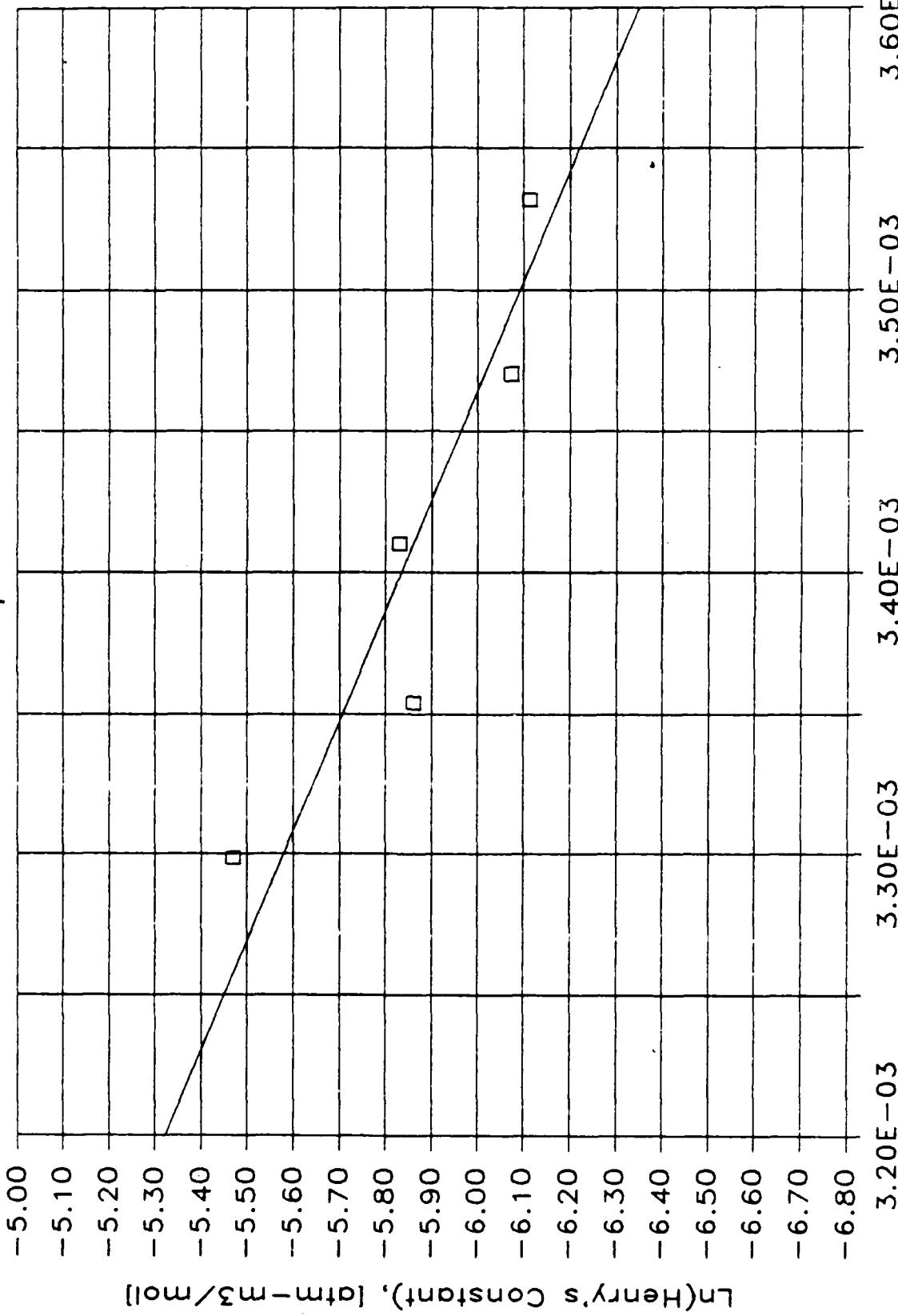
		Temperature 4		Temperature 5	
RUN Number —>		11		9	
REPLICATE —>		No. 1	No. 2	No. 1	No. 2
Group No.		2		2	
Component ID		7		7	
Temperature (C)		25		39	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H _{avg} : atm-m ³ /mol		0.1166	1.0E-25	0.1696	1.0E-25
H _{avg} : atm-mol/mol		158.3		234.2	
H _{avg} : atm-m ³ /mol		2.85E-03	1	4.22E-03	1
H _{avg} : kPa-m ³ /mol		0.2890		0.4276	
COV, r [std/mean]		0.59		4.16	
COV, both replic.		—		—	
Observation: (1)		0.1160		0.1781	
[atm-m ³ /mol]	(2)	0.1160		0.1677	
	(3)	0.1172		0.1714	
	(4)	0.1172		0.1612	
Injection: (1)		824190		1093500	
[Peak Area]	(2)	828310		1069500	
	(3)	3390800		3579100	
	(4)	3390700		3704500	

Temperature Regression Parameters:

OF POINTS = 5
 SLOPE = -2.6E+03
 Y-INTERCEPT = 2.9E+00
 R-SQUARED = 0.8501

TEMPERATURE REGRESSION PLOT

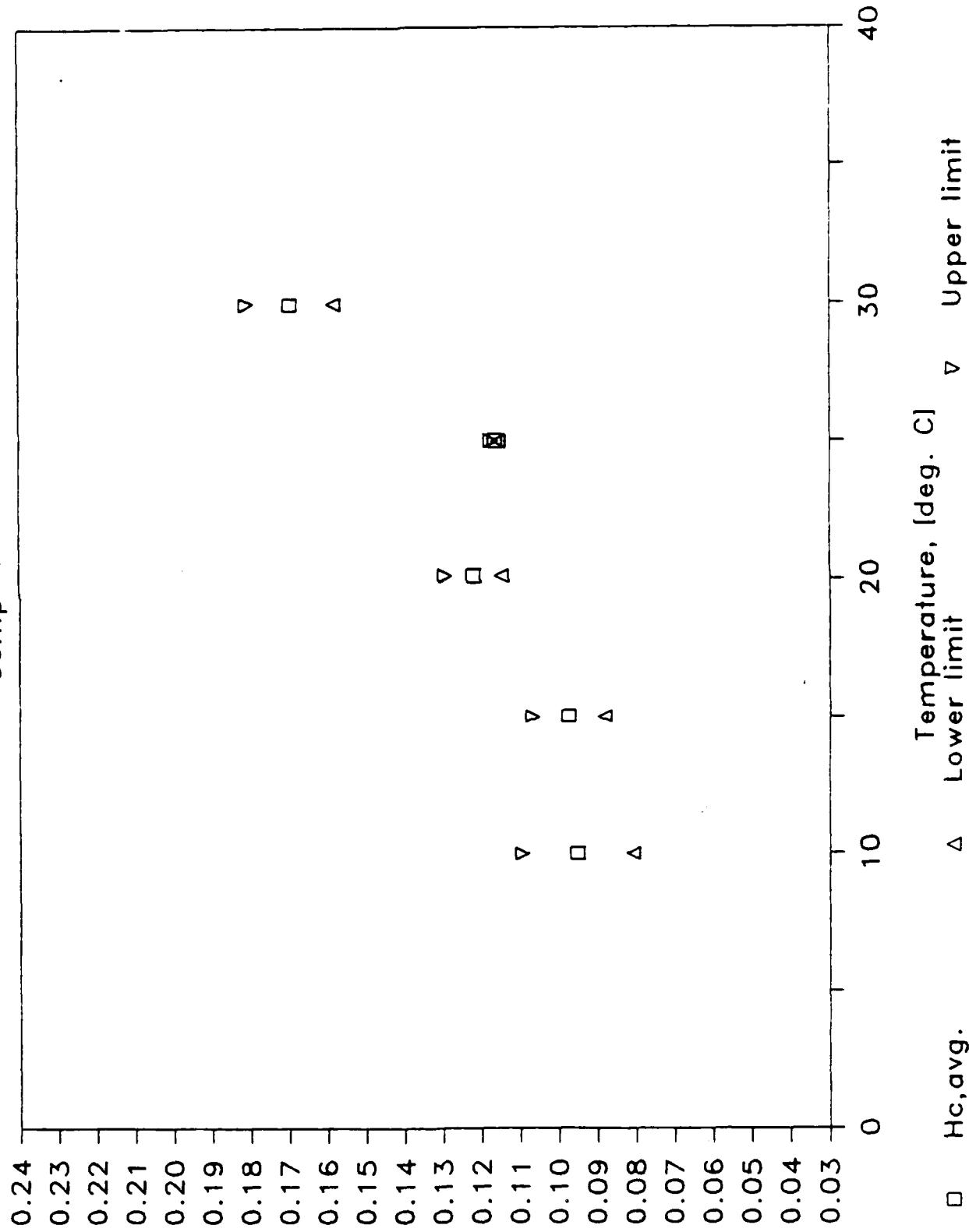
Component 7



□ Experimental data

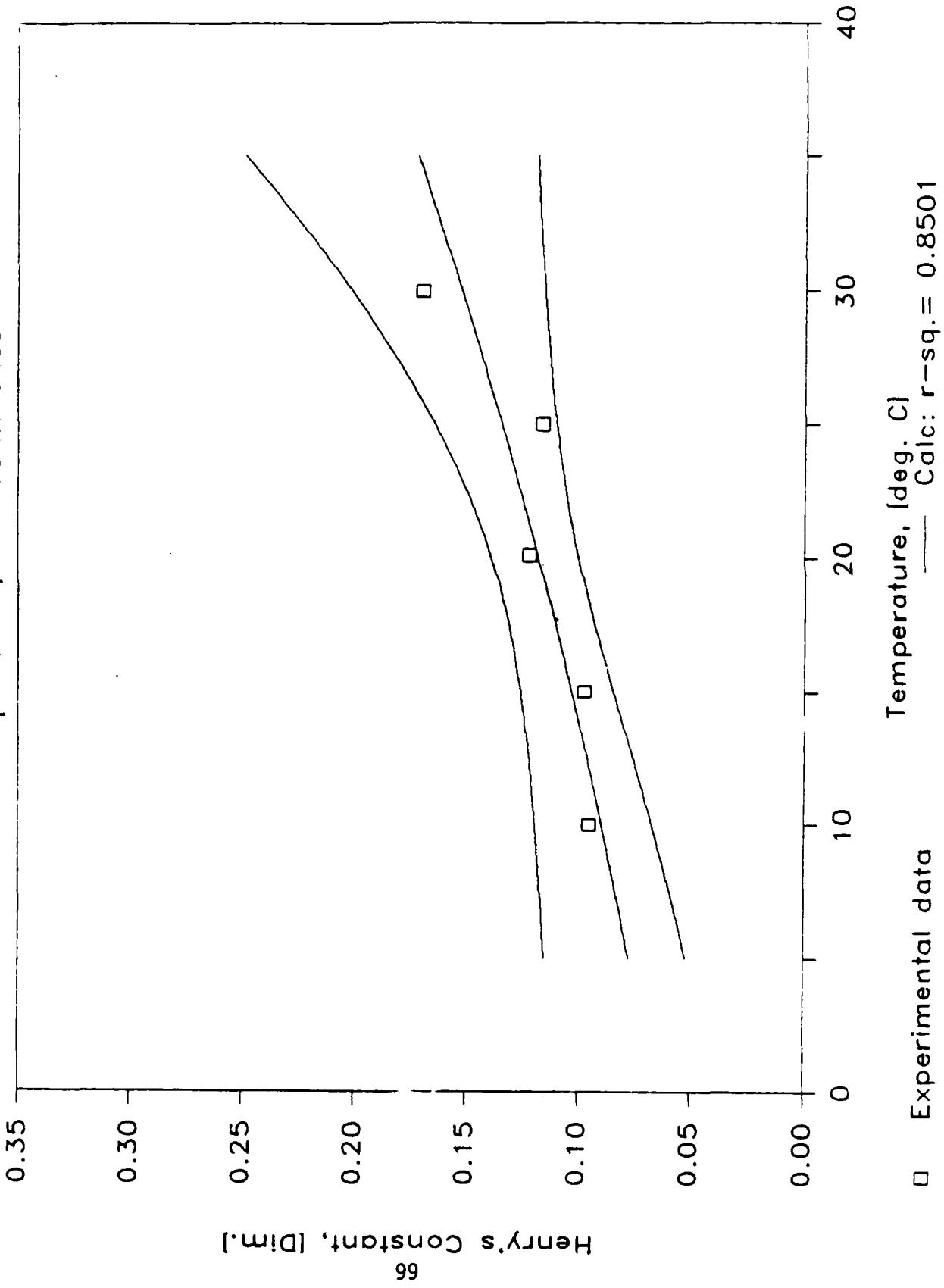
Reciprocal Temperature, [$1/K$] Regr: $r-sq.= 0.8501$

95% CONFIDENCE TEST
Component 7



REGRESSION CONFIDENCE TEST

Component 7, 95% Confidence



04-Nov-86

Results Summary for Component 107

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
REPLICATE —>	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	14		14		14	
Component ID	107		107		107	
Temperature (C)	10.5		15.3		19.5	
Low Vol (ml)	25		25		25	
High Vol (ml)	205		205		205	
System Vol (ml)	250		250		250	
H _{avg} : atm-m ³ /mol	0.0506	1.0E-25	0.0994	1.0E-25	0.1215	1.0E-25
H _{avg} : atm-mol/mol	65.4		130.6		161.9	
H _{avg} : atm-m ³ /mol	1.18E-03	1	2.35E-03	1	2.92E-03	1
H _{avg} : kPa-m ³ /mol	0.1194		0.2384		0.2956	
COV, r [std/mean]	16.52		16.97		19.71	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0607		0.1128		0.1160	
(atm-m ³ /mol)	(2)	0.0478	0.1151		0.1513	
(3)	0.0532		0.0838		0.0935	
(4)	0.0409		0.0858		0.1251	
Injection: (1)	193660		263660		265060	
[Peak Area]	(2)	185550	230970		239940	
(3)	1040900		1099300		1090600	
(4)	1122100		1088800		950770	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		92		80	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		14		14	
Component ID		107		107	
Temperature (C)		25.2		30	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H _c avg: atm-m ³ /mol		0.1231	1.0E-25	0.1501	1.0E-25
H _c avg: atm-mol/mol		167.2		207.2	
H _c avg: atm-m ³ /mol		3.01E-03	1	3.73E-03	1
H _c avg: kPa-m ³ /mol		0.3053		0.3782	
COV, r [std/mean]		20.19		4.92	
COV, both replic.		_____		_____	
Observation: (1)		0.1462		0.1525	
[atm-m ³ /mol]	(2)	0.1429		0.1414	
	(3)	0.1029		0.1588	
	(4)	0.1003		0.1475	
Injection: (1)		419960		578310	
[Peak Area]	(2)	352660		591410	
	(3)	1535000		2065800	
	(4)	1553600		2151100	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

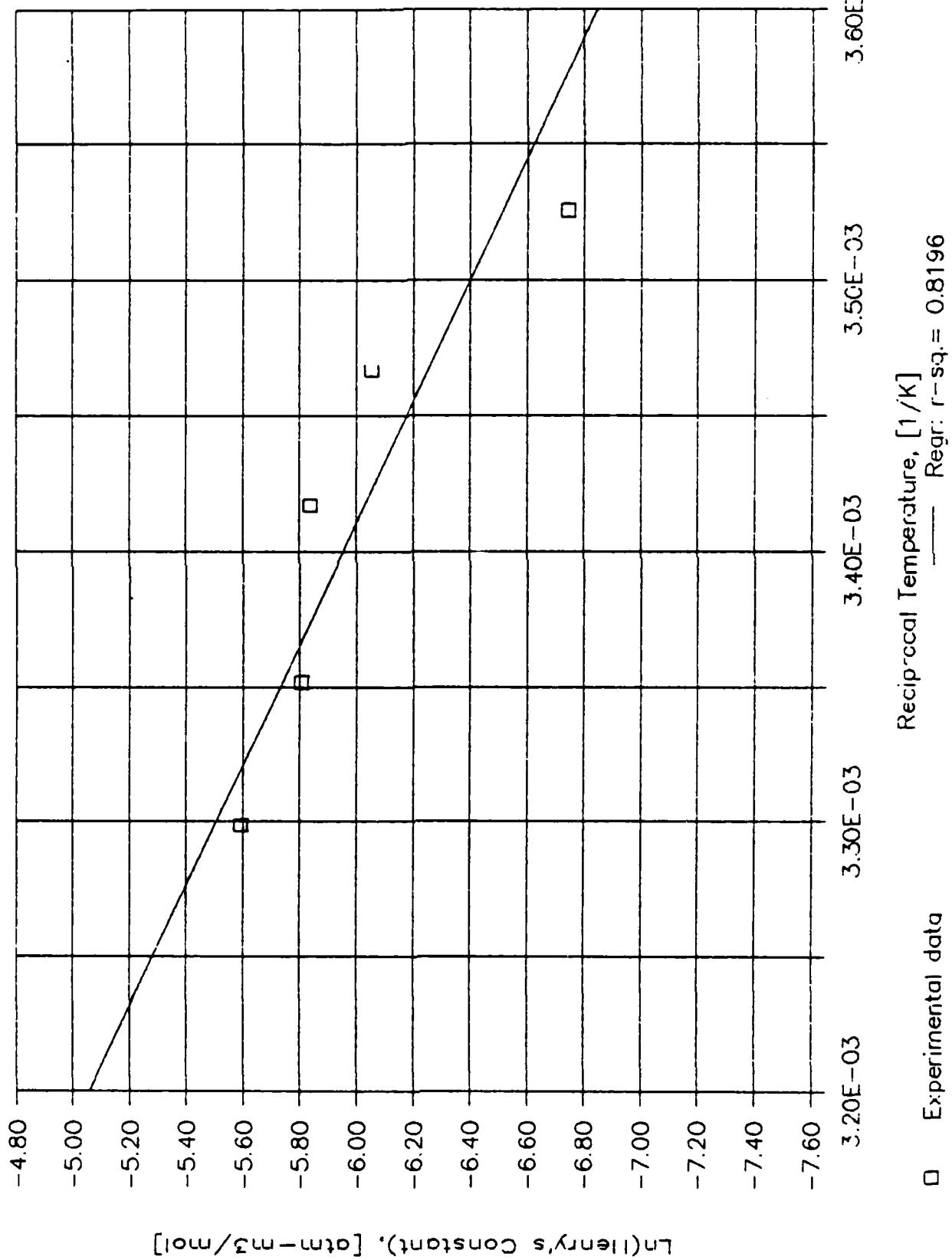
SLOPE = -4.5E+03

Y-INTERCEPT = 9.2E+00

R-SQUARED = 0.8196

TEMPERATURE REGRESSION PLOT

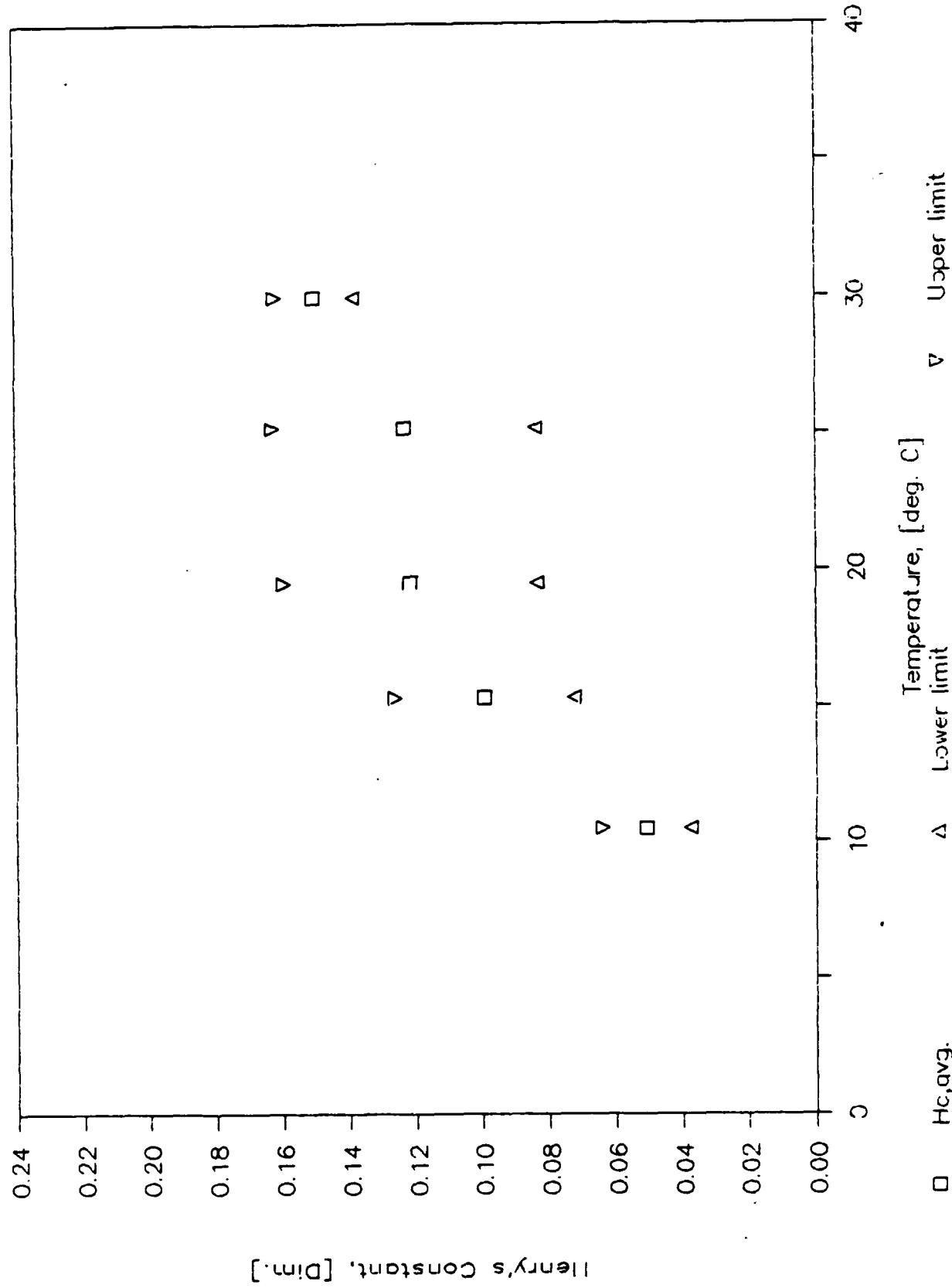
Component 1C7



$\ln(\text{Henry's Constant}) [\text{atm} \cdot \text{m}^3/\text{mol}]$

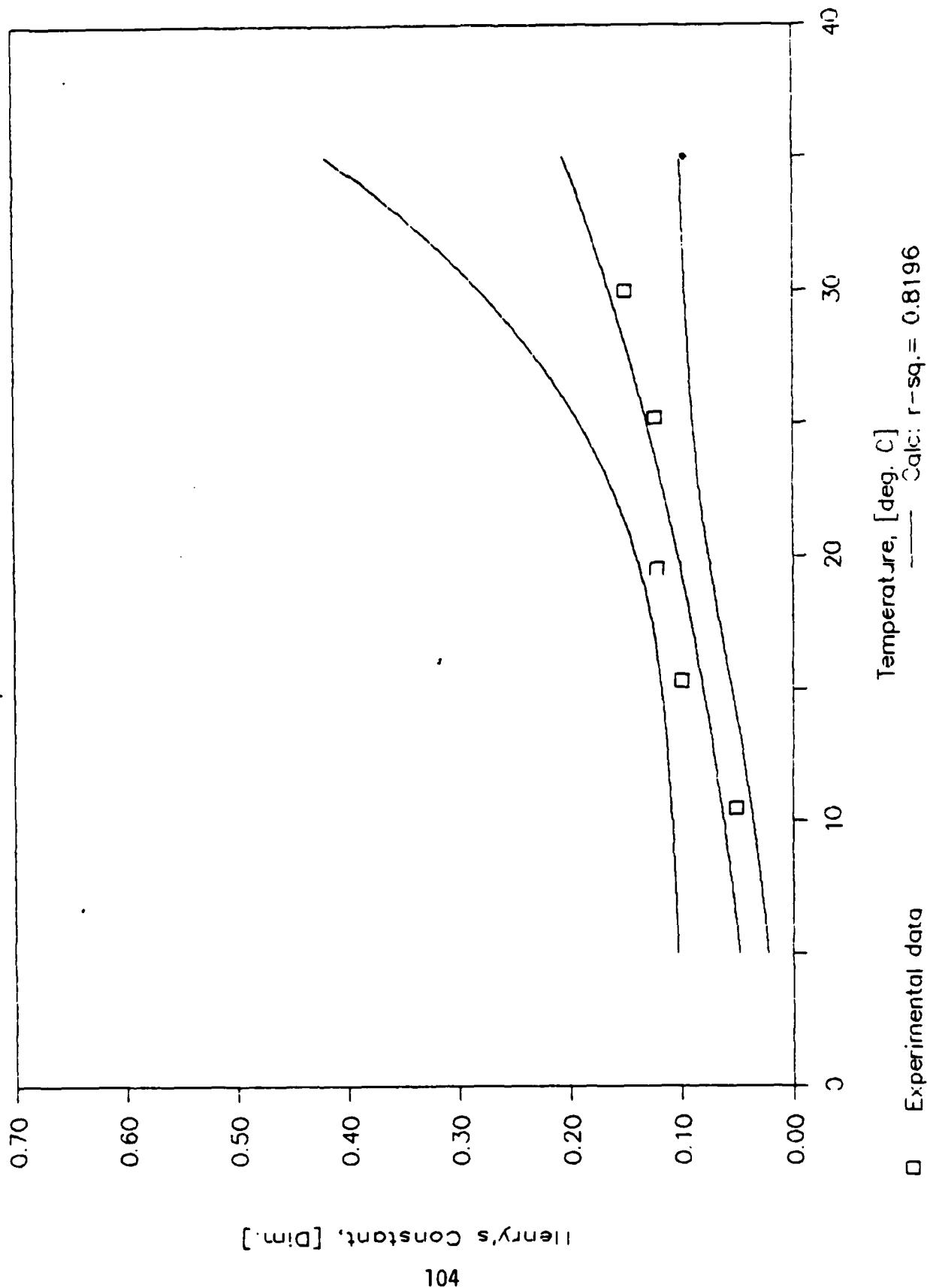
95% CONFIDENCE TEST

Component 1C7



REGRESSION CONFIDENCE TEST

Component 107, 95% Confidence



Henry's Constant, [Dim.]

06-Nov-86

Results Summary for Component 8

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	2		2		2	
Component ID	8		8		8	
Temperature (C)	16		15		20.1	
Low Vol (ml)	25		25		25	
High Vol (ml)	205		205		205	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	0.0912	1.0E-25	0.0918	1.0E-25	0.1075	1.0E-25
H, avg: atm-mol/mol	117.6		129.5		143.6	
H, avg: atm-m3/mol	2.12E-03	1	2.17E-03	1	2.59E-03	1
H, avg: kPa-m3/mol	0.2148		0.2200		0.2622	
COV, r [std/mean]	5.03		5.59		4.08	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0957		0.0965		0.1129	
(atm-m3/mol) (2)	0.0901		0.0960		0.1075	
(3)	0.0923		0.0877		0.1075	
(4)	0.0968		0.0871		0.1022	
Injection: (1)	254220		289000		356620	
(Peak Area) (2)	262270		277250		348390	
(3)	1198800		1295300		1486100	
(4)	1173900		1298800		1521500	

06-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	15	13	13	13
REPLICATE →	No. 1	No. 2	No. 1	No. 2
Group No.	2		2	
Component ID	8		8	
Temperature (C)	25		39	
Low Vol (ml)	25		25	
High Vol (ml)	265		265	
System Vol (ml)	250		250	
H _{avg} : atm-m ³ /mol	0.1296	1.0E-25	0.1563	1.0E-25
H _{avg} : atm-mol/mol	176.0		215.8	
H _{avg} : atm-m ³ /mol	3.17E-03	1	3.89E-03	1
H _{avg} : kPa-m ³ /mol	0.3212		0.3948	
COV, r [std/mean]	8.35		9.17	
COV, both replic.	—		—	
Observation: (1)	0.1428		0.1741	
[atm-m ³ /mol] (2)	0.1273		0.1571	
(3)	0.1315		0.1549	
(4)	0.1167		0.1391	
Injections: (1)	463370		549630	
[Peak Area] (2)	443770		514710	
(3)	1714600		1822700	
(4)	1828400		1931400	

Temperature Regression Parameters:

OF POINTS = 5

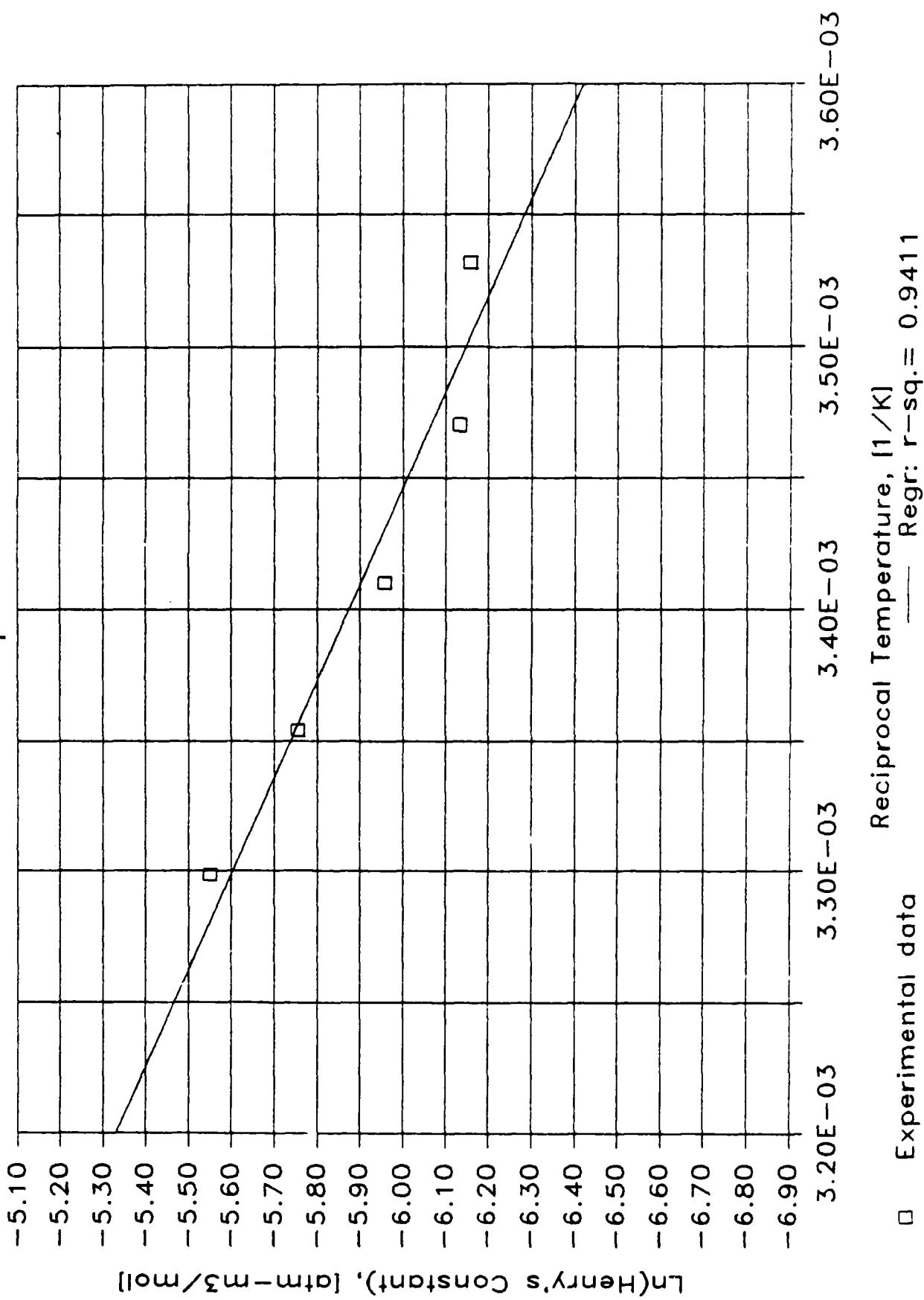
SLOPE = -2.7E+03

Y-INTERCEPT = 3.4E+00

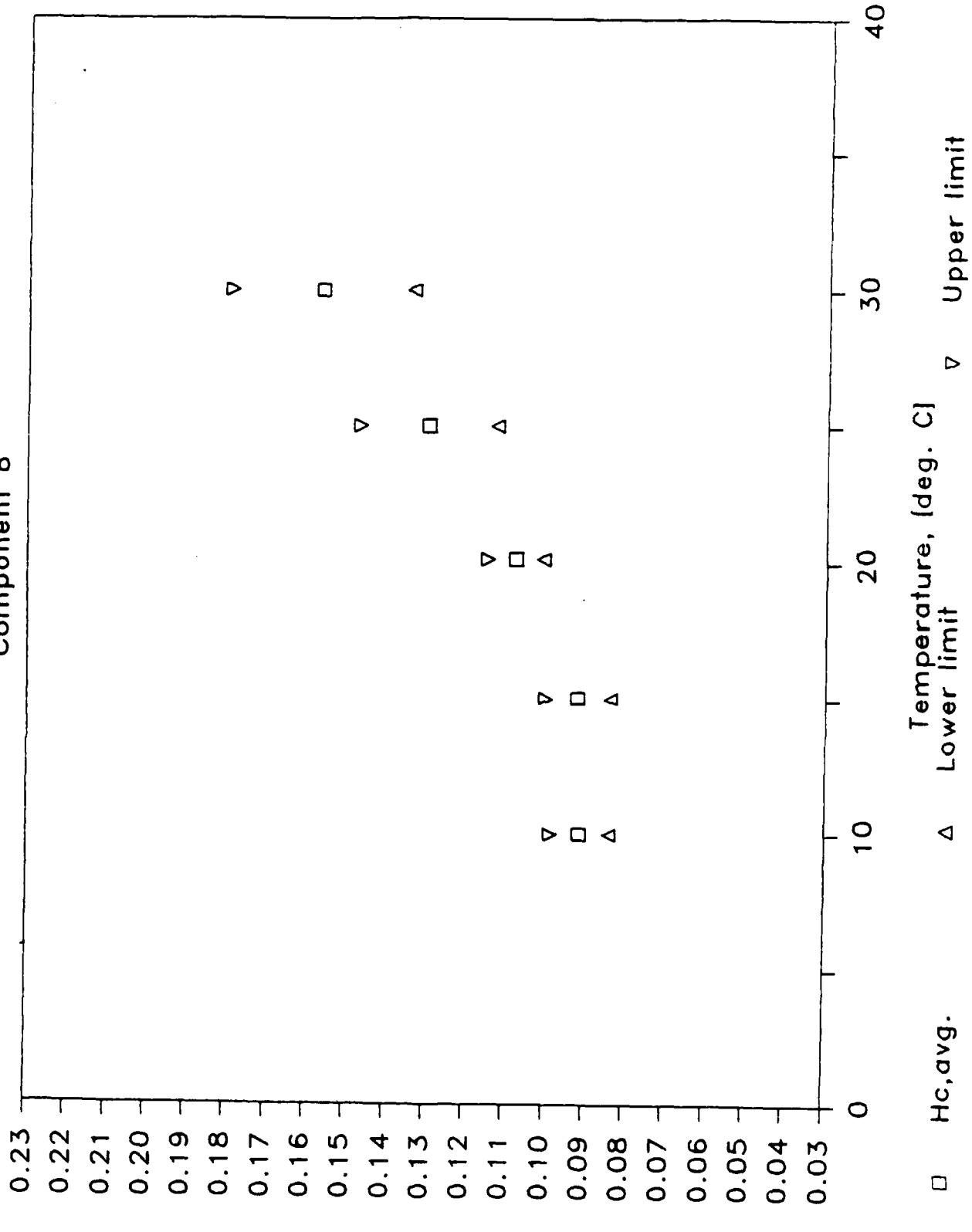
R-SQUARED = 0.9411

TEMPERATURE REGRESSION PLOT

Component 8

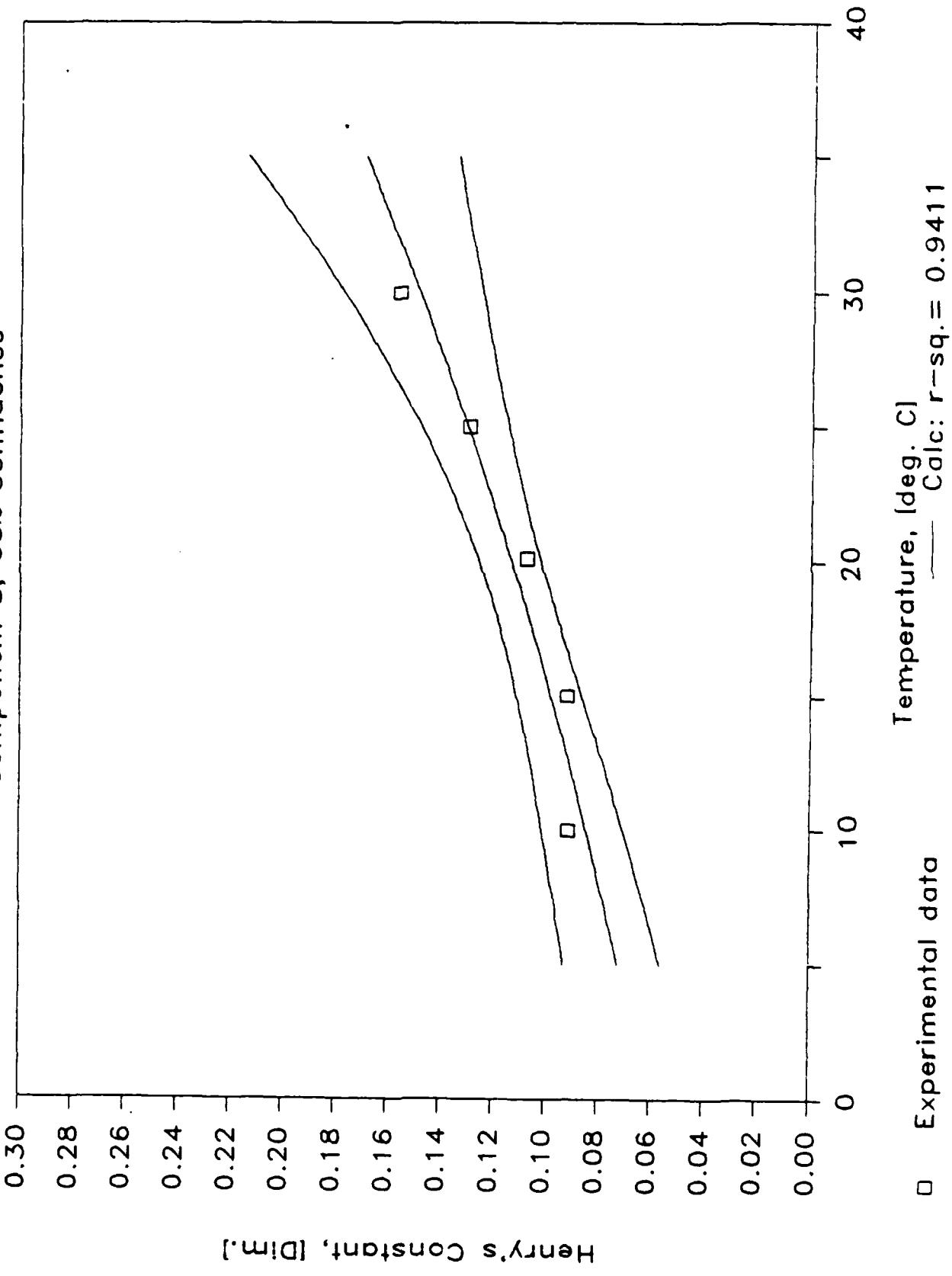


95% CONFIDENCE TEST
Component B



REGRESSION CONFIDENCE TEST

Component 8, 95% Confidence



04-Nov-86

Results Summary for Component 108

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		83		96		107	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		14		14		14	
Component ID		108		108		108	
Temperature (C)		10.5		15.3		19.5	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H, avg: atm-m3/m3		0.0700	1.0E-25	0.0909	1.0E-25	0.1034	1.0E-25
H, avg: atm-mol/mol		90.4		119.5		137.9	
H, avg: atm-m3/mol		1.63E-03	1	2.15E-03	1	2.48E-03	1
H, avg: kPa-m3/mol		0.1650		0.2181		0.2517	
COV, r [std/mean]		21.53		13.64		16.65	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.0778		0.1017		0.1089	
[atm-m3/m3] (2)		0.0868		0.1016		0.1241	
(3)		0.0537		0.0802		0.0837	
(4)		0.0615		0.0801		0.0970	
Injection: (1)		216910		262360		290240	
[Peak Area] (2)		190240		236960		258320	
(3)		1064100		1148300		1230600	
(4)		1017500		1148700		1154800	

04-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4			Temperature 5		
	97		84	No. 1	No. 2	No. 1
REPLICATE →						
Group No.		14			14	
Component ID		108			108	
Temperature (C)		25.2			30	
Low Vol (ml)		25			25	
High Vol (ml)		205			205	
System Vol (ml)		250			250	
H ₄ avg: atm-m ³ /m ³	0.1159	1.0E-25		0.1607	1.0E-25	
H ₄ avg: atm-mol/mol	157.6			221.9		
H ₄ avg: atm-m ³ /mol	2.84E-03	1		4.00E-03	1	
H ₄ avg: kPa-m ³ /mol	0.2876			0.4050		
COV, r [std/mean]	1.69			10.89		
COV, both replic.	_____			_____		
Observation: (1)	0.1171			0.1765		
[atm-m ³ /m ³] (2)	0.1181			0.1461		
(3)	0.1138			0.1752		
(4)	0.1148			0.1450		
Injection: (1)	388280			564590		
[Peak Area] (2)	383020			562200		
(3)	1590200			1858000		
(4)	1583700			2063900		

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

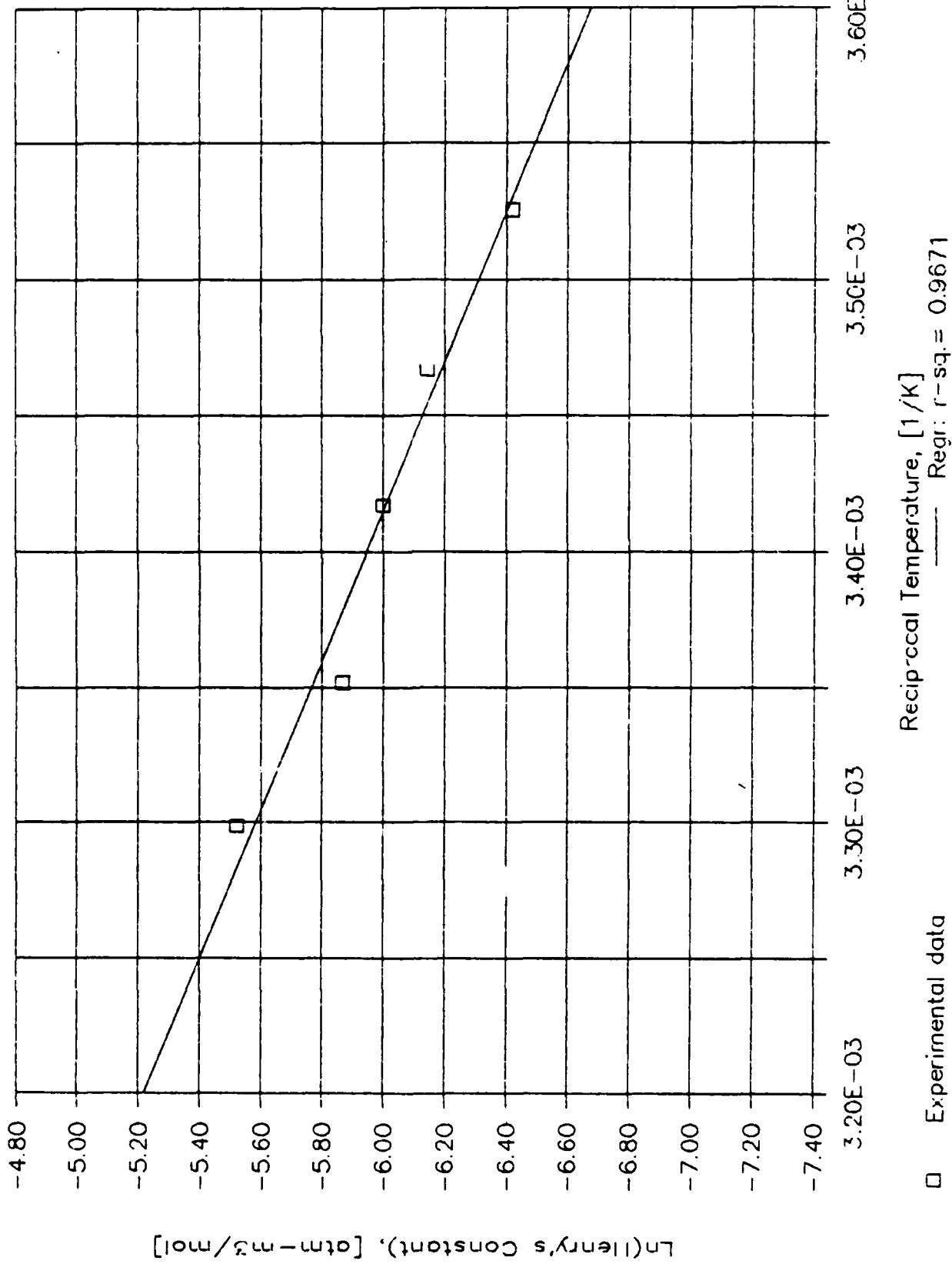
SLOPE = -3.6E+03

Y-INTERCEPT = 6.4E+00

R-SQUARED = 0.9671

TEMPERATURE REGRESSION PLOT

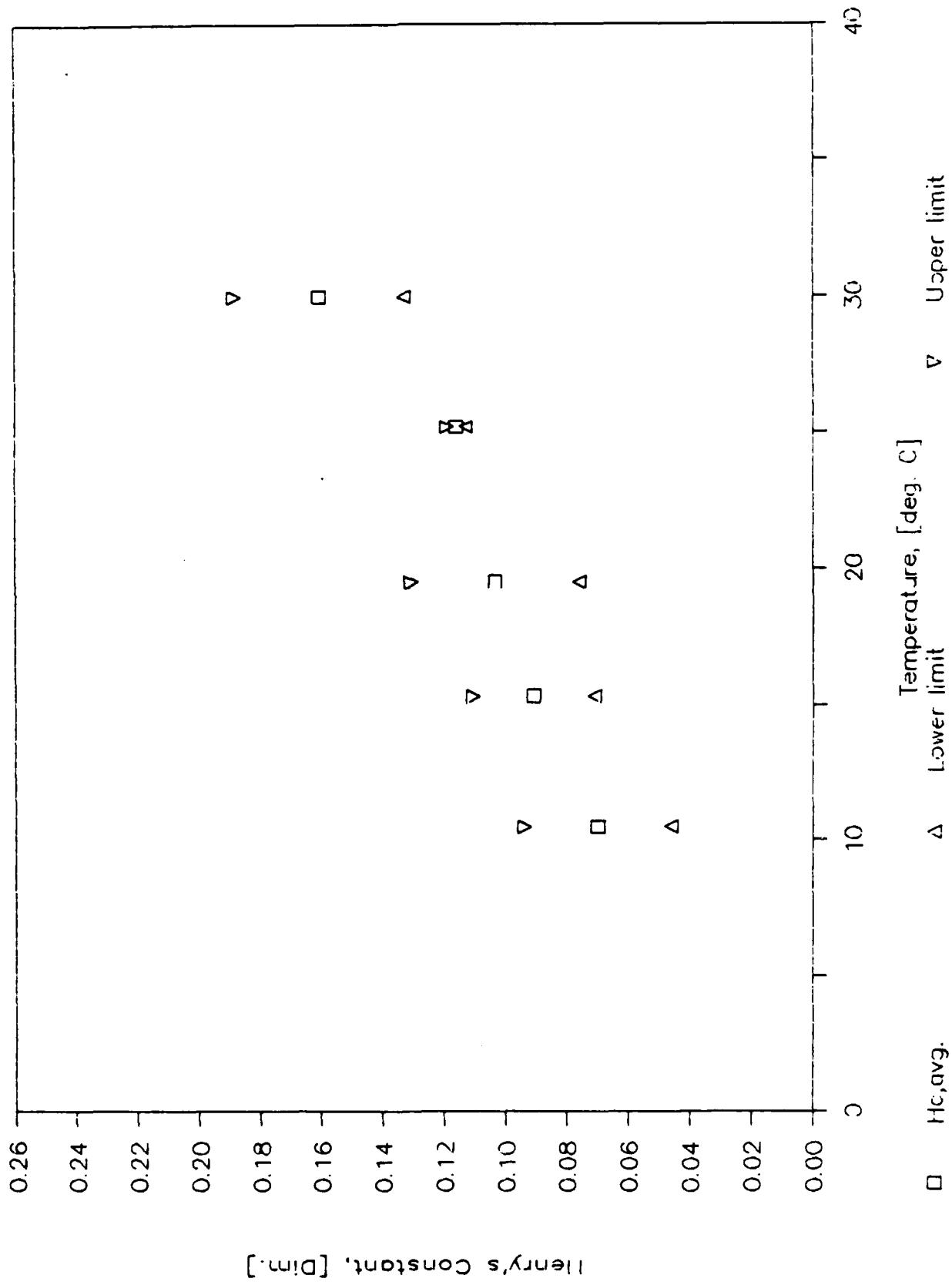
Component 1C8



Ln (Henry's Constant), [atm-m³/mol]

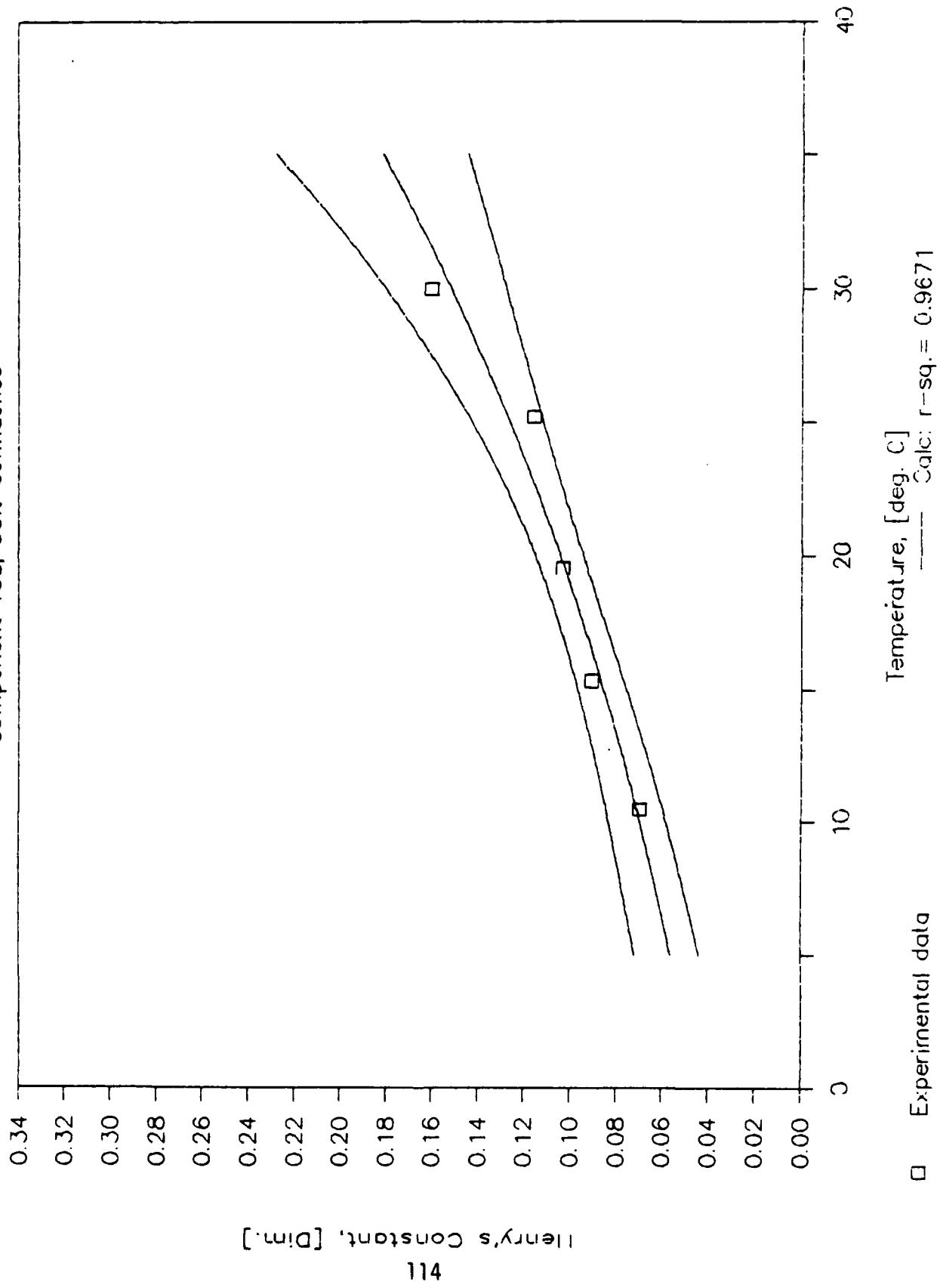
95% CONFIDENCE TEST

Component 1C8



REGRESSION CONFIDENCE TEST

Component 108, 95% Confidence



06-Nov-86

Results Summary for Component 9

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
	2	No. 1 No. 2	1	No. 1 No. 2	2	No. 1 No. 2
REPLICATE —>						
Group No.		3		3		3
Component ID		9		9		9
Temperature (C)		10		15		20.2
Low Vol (ml)		30		30		30
High Vol (ml)		210		210		210
System Vol (ml)		250		250		250
H _c avg: atm-m ³ /mol	0.1228	1.0E-25	0.1528	1.0E-25	0.1969	1.0E-25
H _c avg: atm-mol/mol	158.4		200.6		263.1	
H _c avg: atm-m ³ /mol	2.85E-03	1	3.61E-03	1	4.74E-03	1
H _c avg: kPa-m ³ /mol	0.2891		0.3661		0.4893	
COV, r [std/mean]	5.30		5.04		5.62	
COV, both replic.	—	—	—	—	—	—
Observation: (1)	0.1207		0.1519		0.2041	
[atm-m ³ /mol] (2)	0.1305		0.1623		0.2084	
(3)	0.1152		0.1435		0.1855	
(4)	0.1248		0.1536		0.1896	
Injection: (1)	427950		545320		695270	
[Peak Area] (2)	419230		530300		659600	
(3)	1625900		1858200		2025300	
(4)	1568600		1796800		2001300	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number —>		3		12	
REPLICATE —>		No. 1	No. 2	No. 1	No. 2
Group No.		3		3	
Component ID		9		9	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H ₄ avg: atm-m ³ /mol		0.1989	1.0E-25	0.2516	1.0E-25
H ₄ avg: atm-mol/mol		270.1		347.5	
H ₄ avg: atm-m ³ /mol		4.87E-03	1	6.26E-03	1
H ₄ avg: kPa-m ³ /mol		0.4930		0.6343	
COV, r [std/mean]		2.11		1.93	
COV, both replic.		—		—	
Observations: (1)		0.2806		0.2459	
[atm-m ³ /mol]	(2)	0.2937		0.2501	
	(3)	0.1940		0.2531	
	(4)	0.1971		0.2574	
Injection:	(1)	826730		1048900	
[Peak Area]	(2)	811700		1057300	
	(3)	2431700		2741800	
	(4)	2410500		2714800	

Temperature Regression Parameters:

OF POINTS = 5

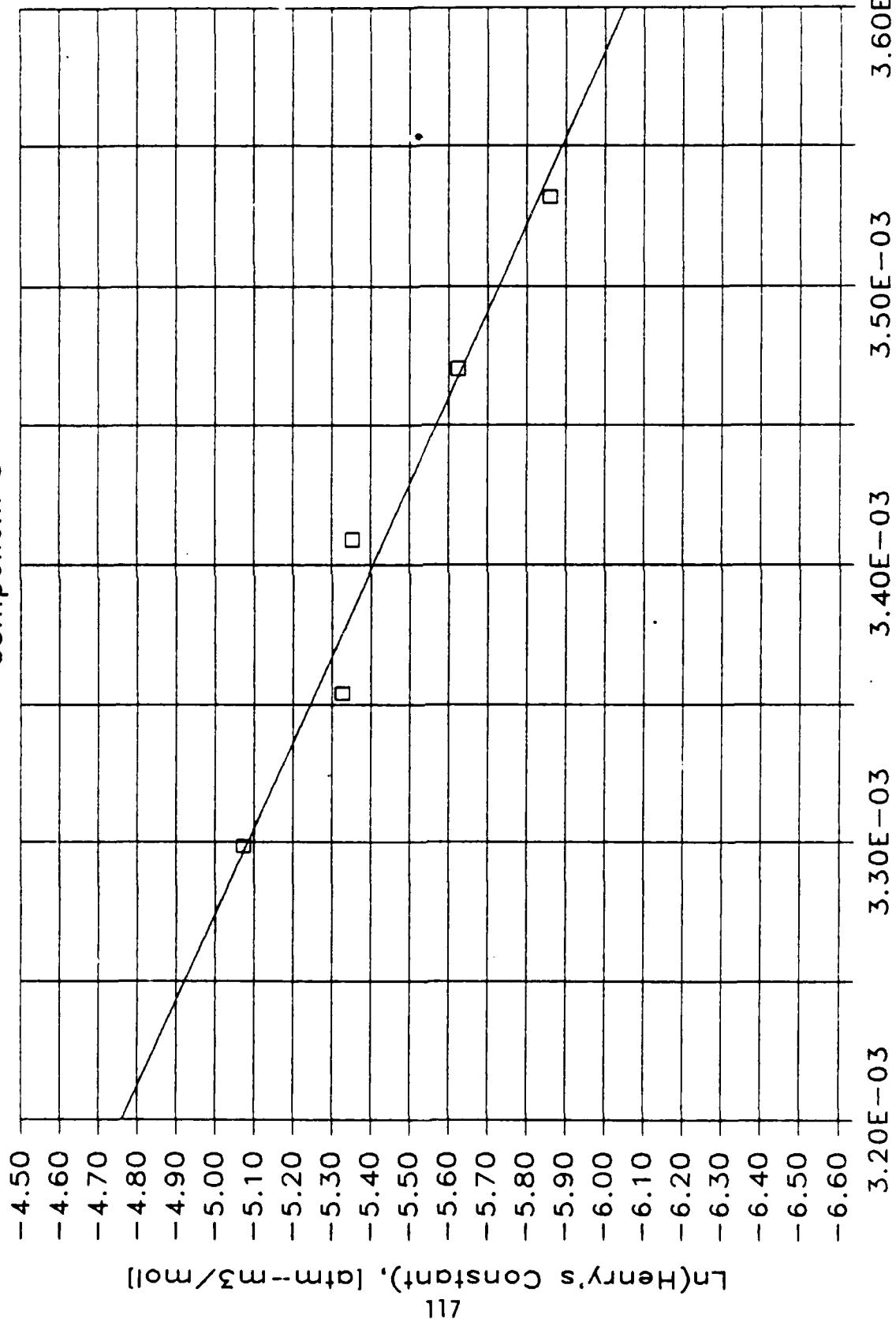
SLOPE = -3.2E+03

Y-INTERCEPT = 5.5E+00

R-SQUARED = 0.9659

TEMPERATURE REGRESSION PLOT

Component 9

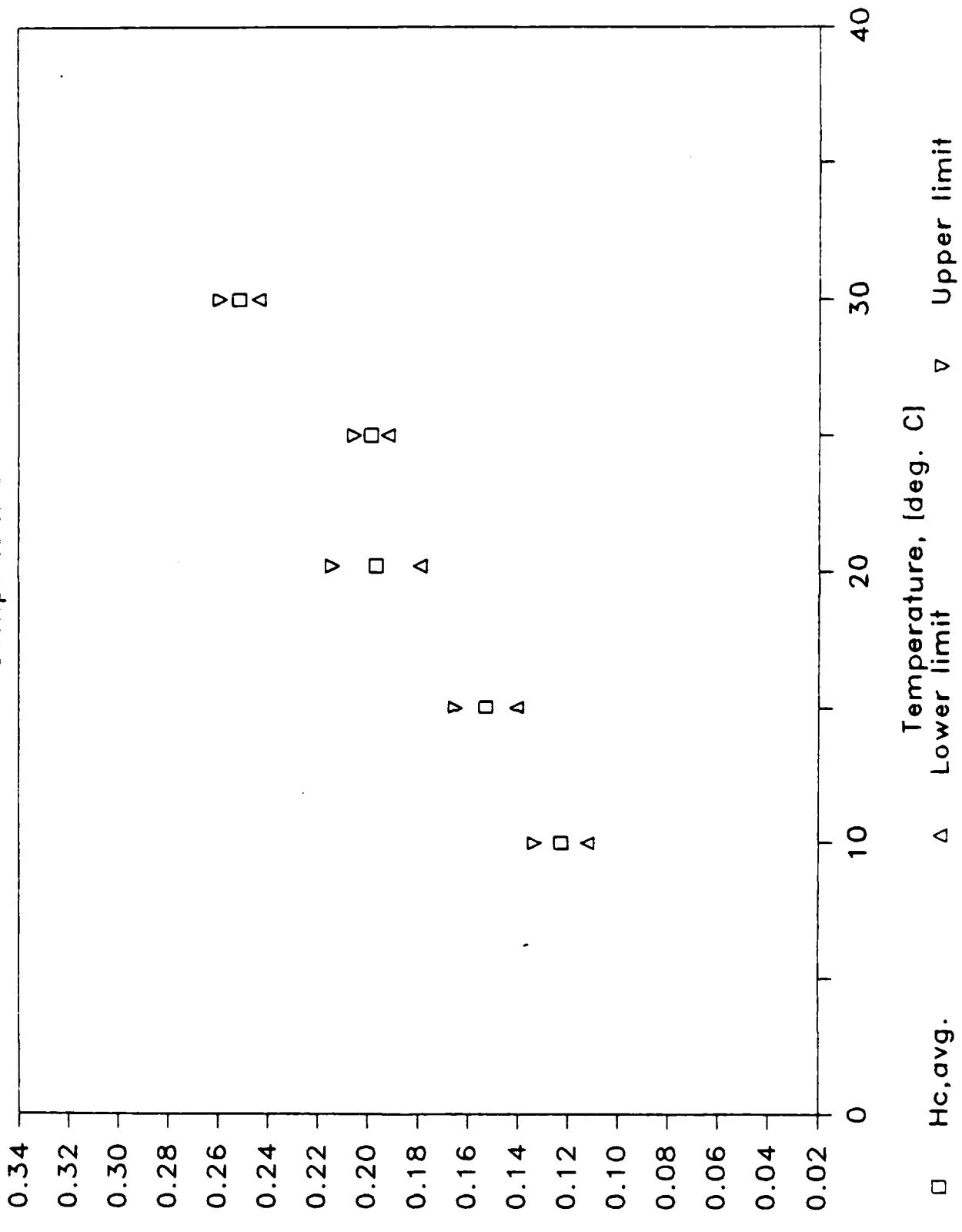


□ Experimental data

Reciprocal Temperature, $[1/\text{K}]$ Regr: $r-sq = 0.9659$

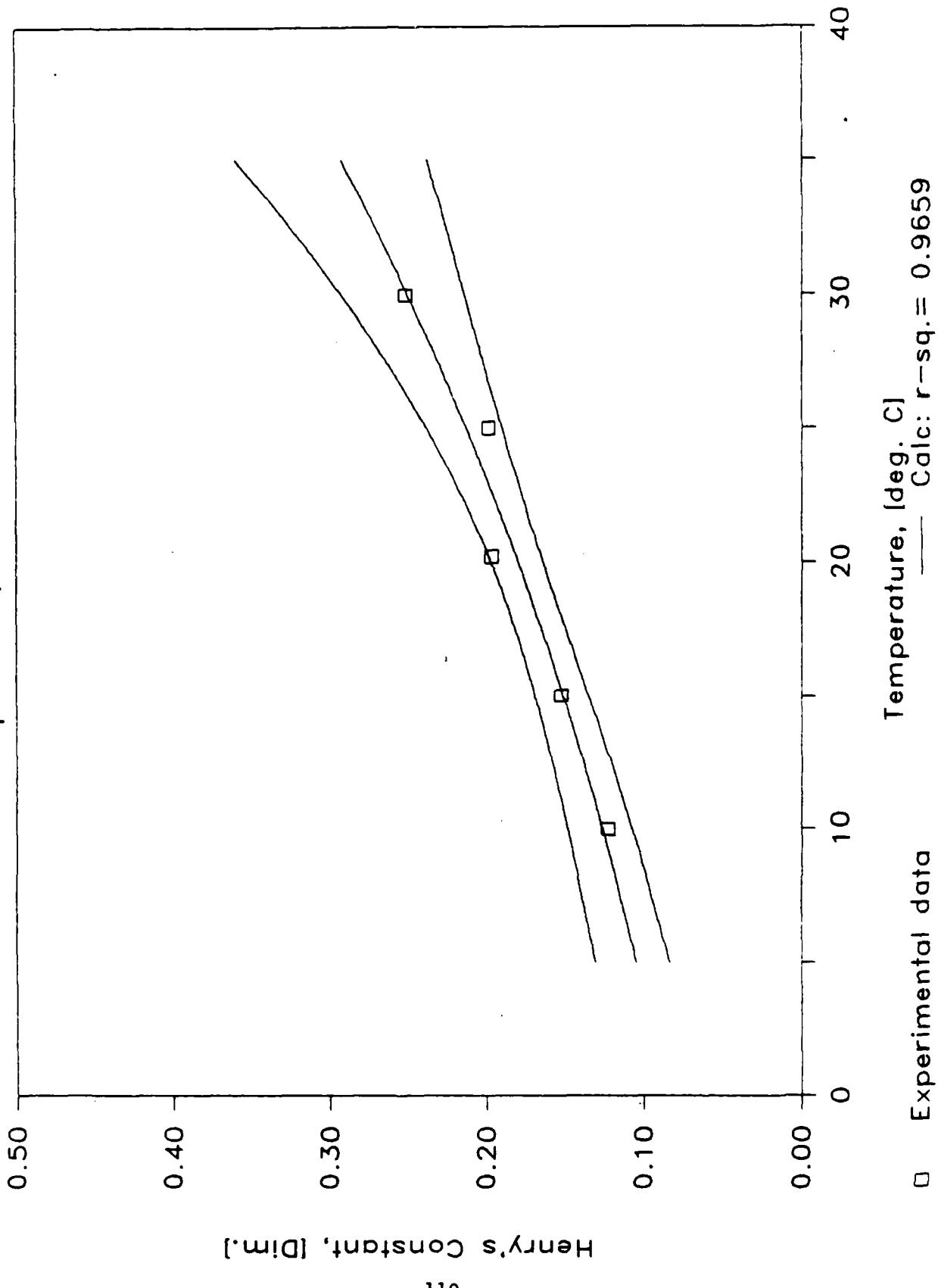
95% CONFIDENCE TEST

Component 9



REGRESSION CONFIDENCE TEST

Component 9, 95% Confidence



06-Nov-86

Results Summary for Component 10

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	6		5		6	
REPLICATE -->	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	3		3		3	
Component ID	10		10		10	
Temperature (C)	10		15		20.2	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H _c avg: atm-m ³ /mol	0.1889	1.0E-25	0.2044	1.0E-25	0.2680	1.0E-25
H _c avg: atm-mol/mol	233.3		268.2		358.1	
H _c avg: atm-m ³ /mol	4.20E-03	1	4.83E-03	1	6.45E-03	1
H _c avg: kPa-m ³ /mol	0.4259		0.4897		0.6537	
COV, r [std/mean]	5.18		4.13		2.51	
COV, both replic.						
Observation: (1)	0.1839		0.2036		0.2624	
[atm-m ³ /mol] (2)	0.1920		0.2148		0.2741	
(3)	0.1699		0.1942		0.2620	
(4)	0.1777		0.2050		0.2736	
Injection: (1)	578570		718850		884190	
[Peak Area] (2)	547100		699270		883270	
(3)	1760100		2094200		2222300	
(4)	1719100		2031800		2163800	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		7		14	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		3		3	
Component ID		10		10	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.3041	1.0E-25	0.3798	1.0E-25
H, avg: atm-mol/mol		412.9		524.4	
H, avg: atm-m3/mol		7.44E-03	1	9.45E-03	1
H, avg: kPa-m3/mol		0.7538		0.9572	
COV, r [std/mean]		1.90		2.14	
COV, both replic.		—		—	
Observation: (1)		0.2909		0.3821	
[atm-m3/m3] (2)		0.3009		0.3895	
(3)		0.2992		0.3702	
(4)		0.3093		0.3773	
Injection: (1)		1078900		1336700	
[Peak Area] (2)		1079000		1308600	
(3)		2501000		2639900	
(4)		2449200		2606600	

Temperature Regression Parameters:

OF POINTS = 5

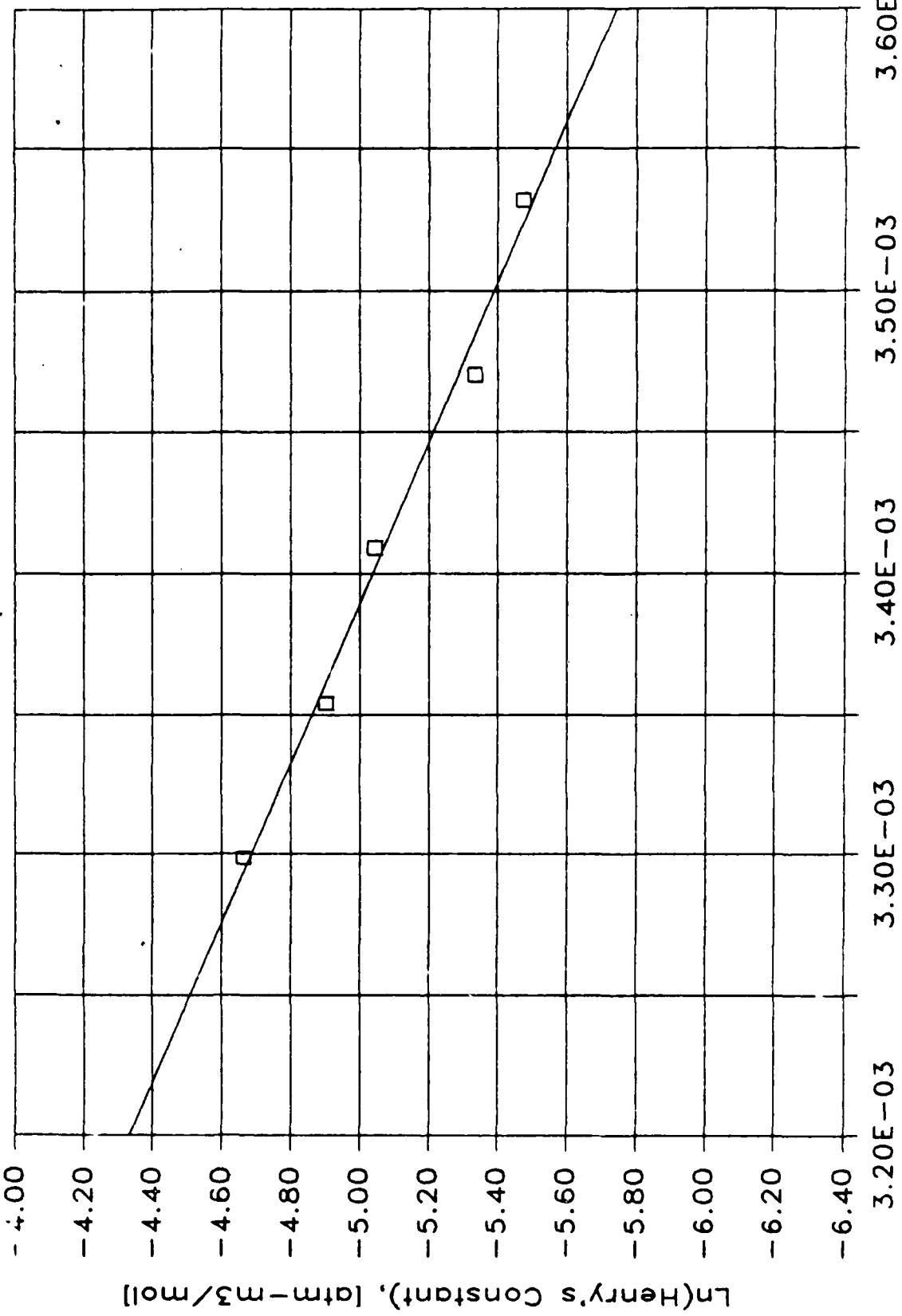
SLOPE = -3.5E+03

Y-INTERCEPT = 6.9E+00

R-SQUARED = 0.9889

TEMPERATURE REGRESSION PLOT

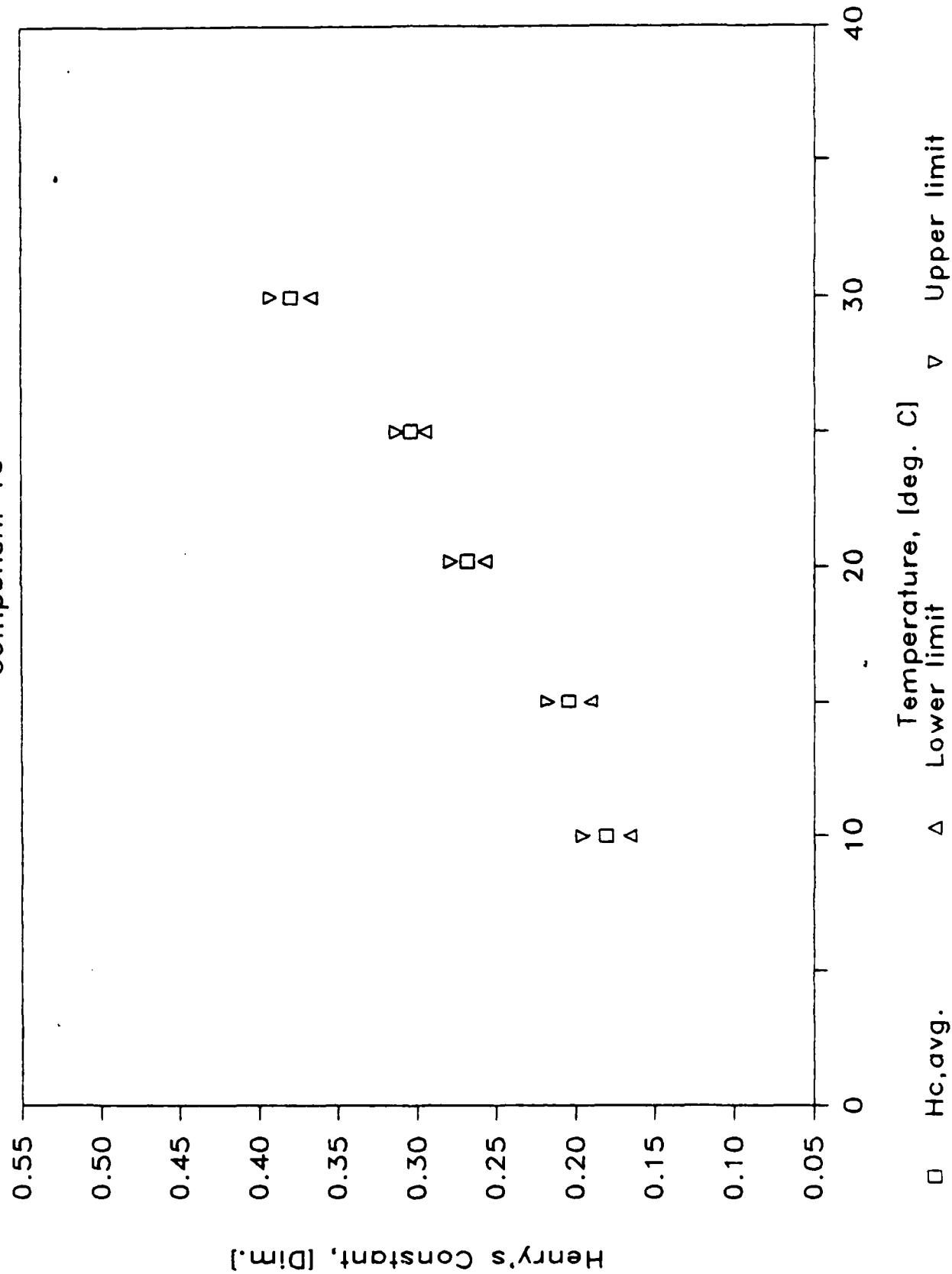
Component 10



□ Experimental data

— Reciprocal Temperature, $(1/\text{K})$
Regr: $r-\text{sq.} = 0.9889$

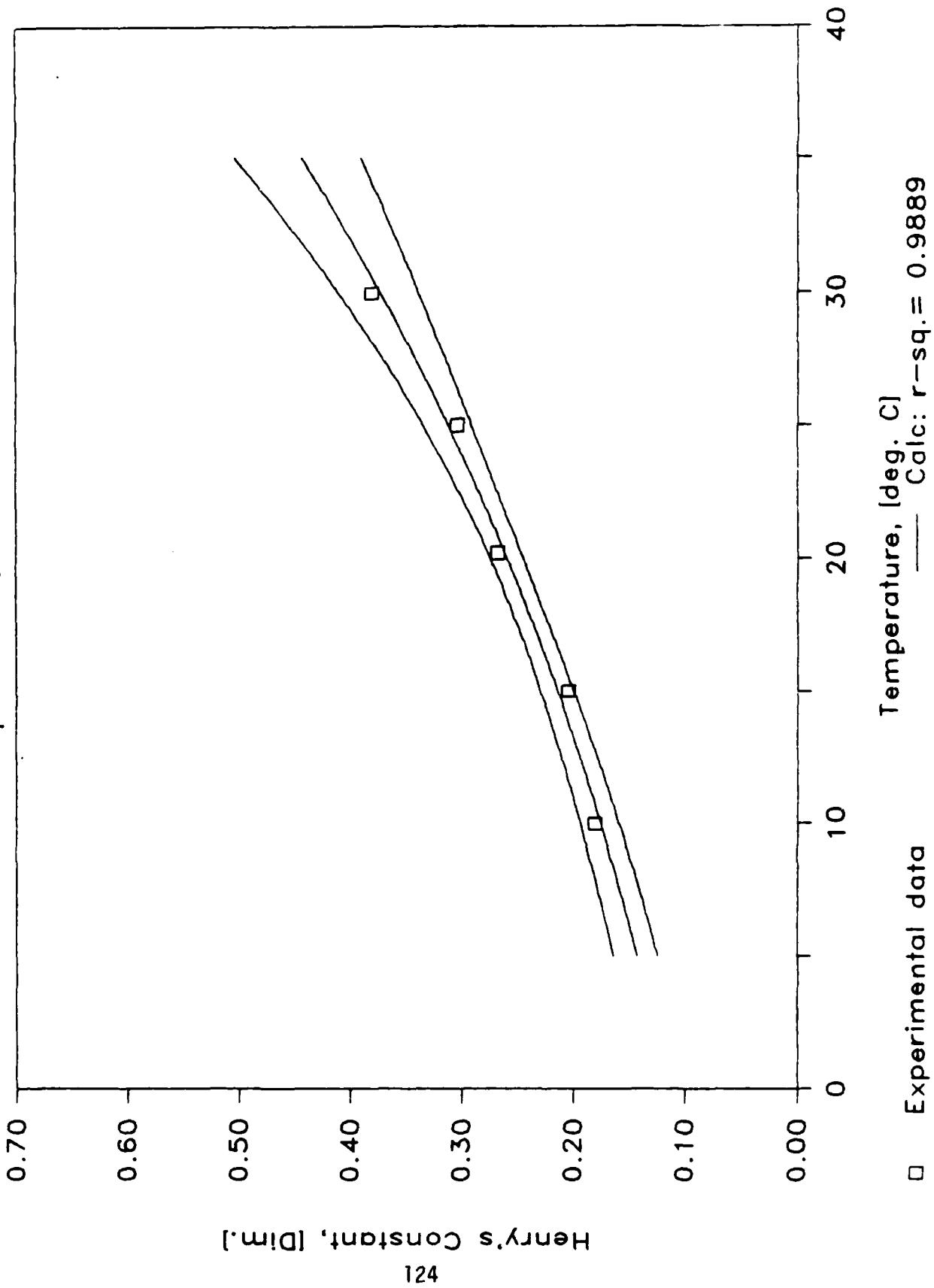
95% CONFIDENCE TEST
Component 10



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 10, 95% Confidence



06-Nov-86

Results Summary for Component 11

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	3		3		3	
Component ID	11		11		11	
Temperature (C)	18		15		20.2	
Low Vol (ml)	38		38		38	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	0.1768	1.0E-25	0.2099	1.0E-25	0.2483	1.0E-25
H, avg: atm-mol/mol	228.0		275.4		331.8	
H, avg: atm-m3/mol	4.11E-03	1	4.96E-03	1	5.98E-03	1
H, avg: kPa-m3/mol	0.4161		0.5028		0.6057	
COV, r [std/mean]	4.71		2.31		3.81	
COV, both replic.	_____		_____		_____	
Observations: (1)	0.1839		0.2095		0.2464	
[atm-m3/mol] (2)	0.1841		0.2158		0.2573	
(3)	0.1694		0.2039		0.2394	
(4)	0.1696		0.2102		0.2501	
Injection: (1)	539200		671850		828900	
[Peak Area] (2)	516360		661730		814790	
(3)	1663800		1928200		2164100	
(4)	1662800		1895800		2108200	

06-Nov-86

Results Summary (continued)

RUN Number —>	Temperature 4			Temperature 5		
	11		17	No. 1		No. 2
REPLICATE —>	No. 1	No. 2		No. 1	No. 2	
Group No.	3			3		
Component ID	11			11		
Temperature (C)	25			39		
Low Vol (ml)	30			30		
High Vol (ml)	210			210		
System Vol (ml)	250			250		
H _{avg} : atm-m ³ /mol	0.3841	1.0E-25		0.3567	1.0E-25	
H _{avg} : atm-mol/mol	413.0			492.5		
H _{avg} : atm-m ³ /mol	7.44E-03	1		8.87E-03	1	
H _{avg} : kPa-m ³ /mol	0.7538			0.8991		
COV, r [std/mean]	4.67			2.50		
COV, both replic.	—			—		
Observation: (1)	0.2956			0.3550		
[atm-m ³ /mol] (2)	0.3194			0.3675		
(3)	0.2890			0.3460		
(4)	0.3124			0.3583		
Injection: (1)	1030200			1201800		
[Peak Area] (2)	1015600			1181700		
(3)	2404700			2492700		
(4)	2288900			2436800		

Temperature Regression Parameters:

OF POINTS = 5

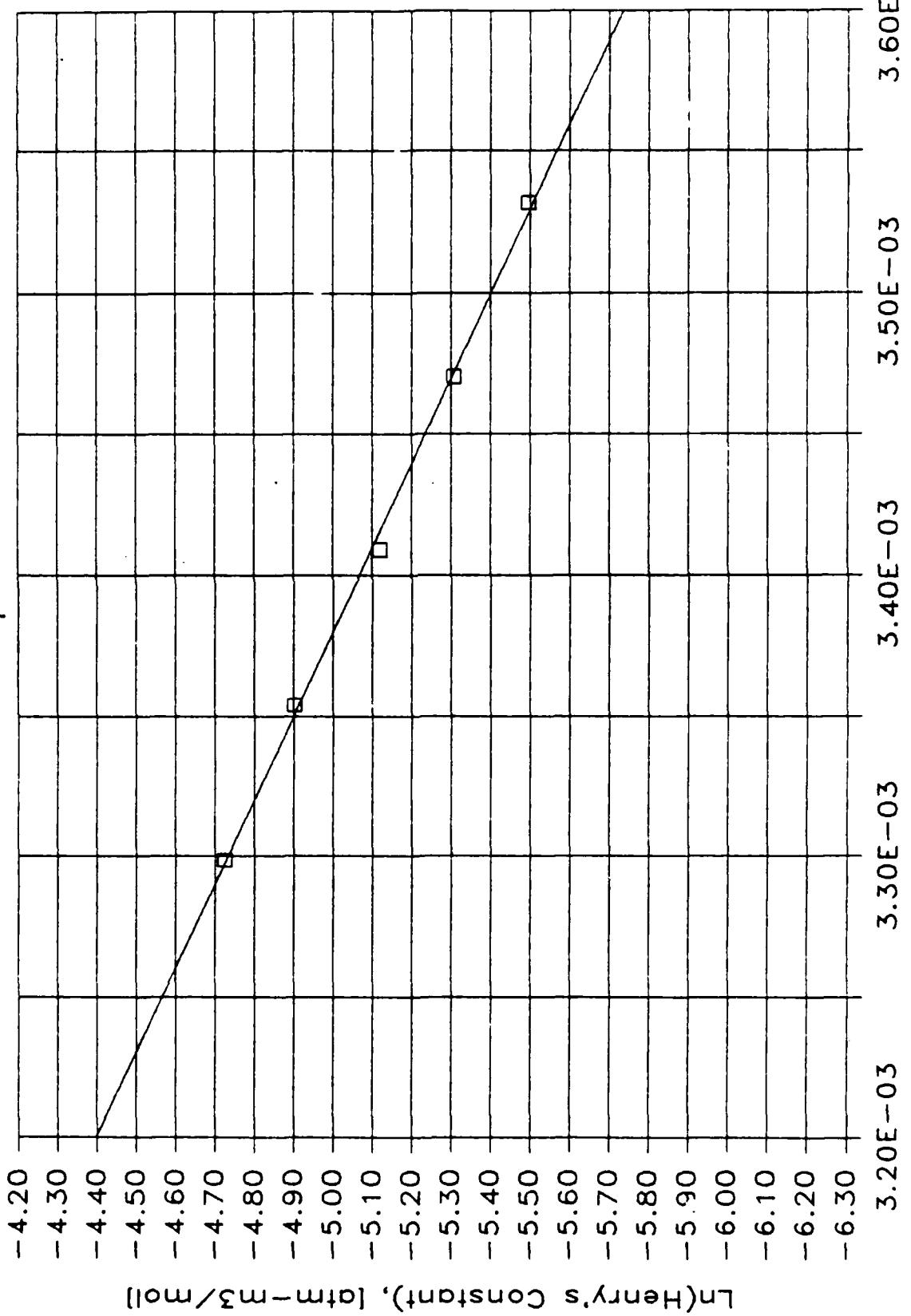
SLOPE = -3.3E+03

Y-INTERCEPT = 6.3E+00

R-SQUARED = 0.9978

TEMPERATURE REGRESSION PLOT

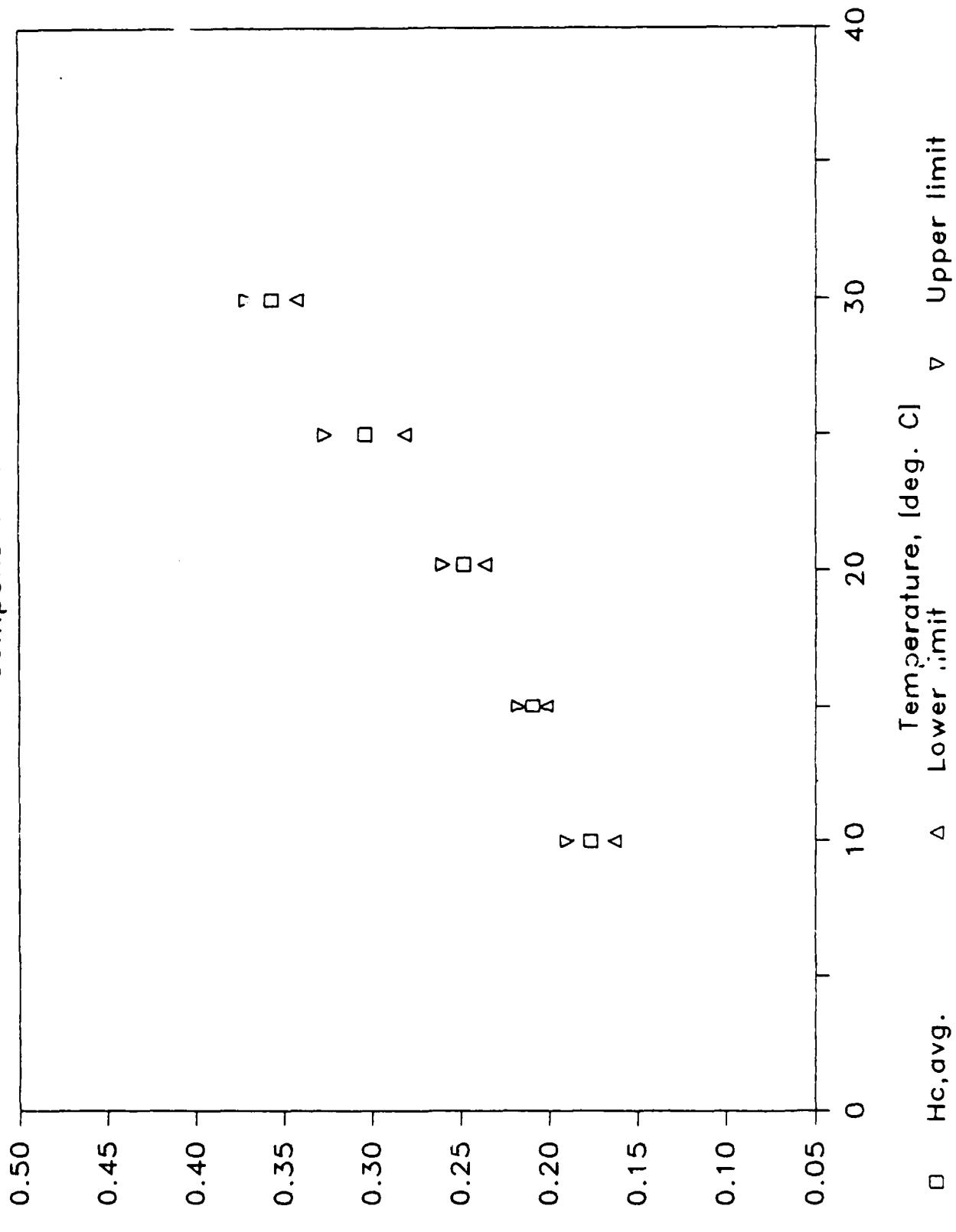
Component 11



□ Experimental data

— Reciprocal Temperature, [1/K]
Regr: r_{sq.} = 0.9978

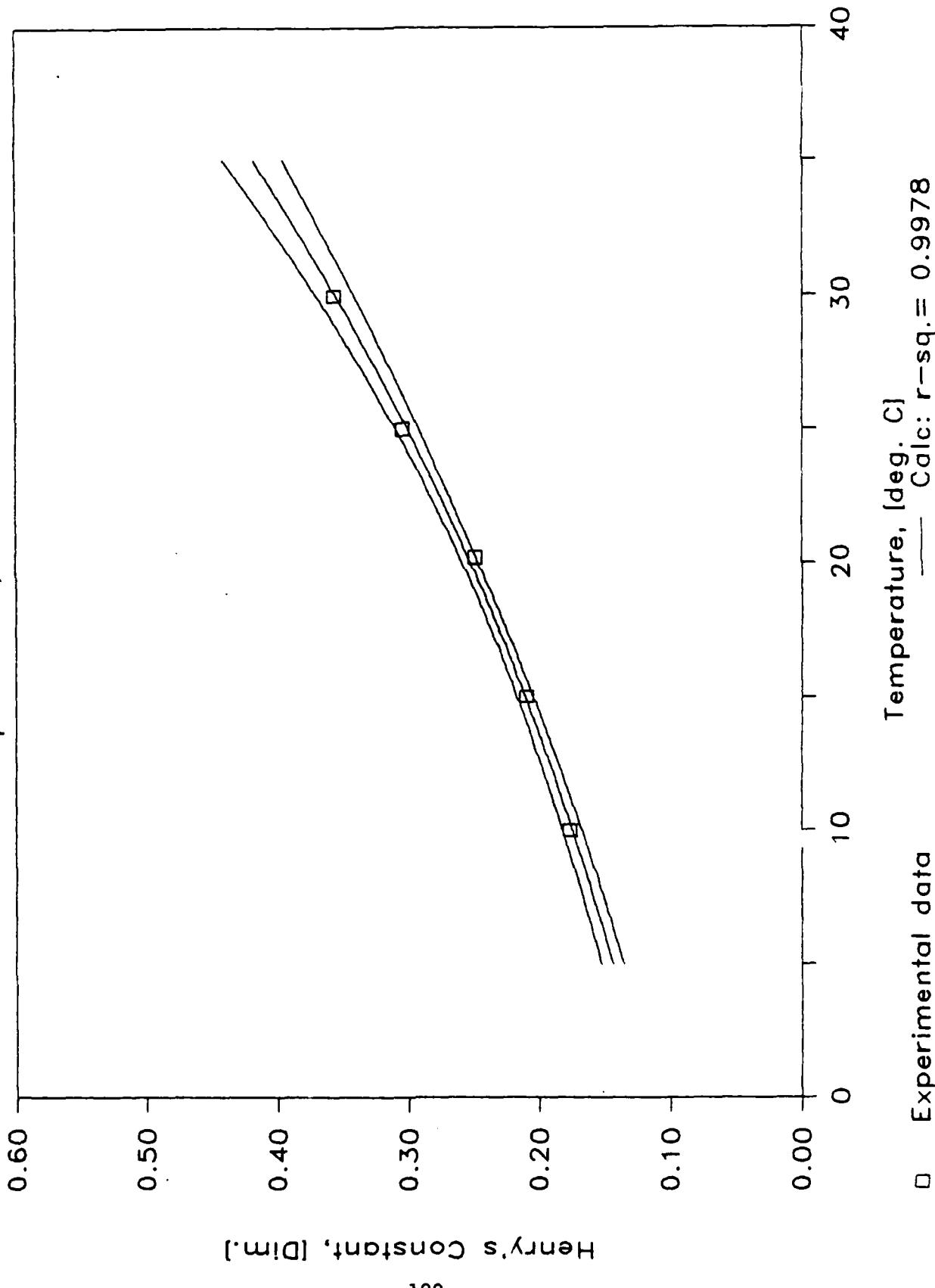
95% CONFIDENCE TEST
Component 11



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 11, 95% Confidence



06-Nov-86

Results Summary for Component 12

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE →						
Group No.	3		3		3	
Component ID	12		12		12	
Temperature (C)	10		15		20.2	
Low Vol (ml)	38		38		38	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	0.2445	1.0E-25	0.3091	1.0E-25	0.3659	1.0E-25
H, avg: atm-mol/mol	315.3		485.7		489.0	
H, avg: atm-m3/mol	5.68E-03	1	7.31E-03	1	8.81E-03	1
H, avg: kPa-m3/mol	0.5756		0.7407		0.8926	
COV, r [std/mean]	3.45		4.82		1.24	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.2390		0.3102		0.3715	
[atm-m3/mol] (2)	0.2533		0.3275		0.3659	
(3)	0.2357		0.2911		0.3660	
(4)	0.2499		0.3076		0.3604	
Injection: (1)	236500		300360		362820	
[Peak Area] (2)	234600		288510		359210	
(3)	628850		679910		730160	
(4)	607340		656600		737630	

06-Nov-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	15	20	15	20
REPLICATE -->	No. 1	No. 2	No. 1	No. 2
Group No.	3		3	
Component ID	12		12	
Temperature (C)	25		38	
Low Vol (ml)	38		38	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H ₄ avg: atm-m ³ /m ³	0.4399	1.0E-25	0.5582	1.0E-25
H ₄ avg: atm-mol/mol	597.4		759.7	
H ₄ avg: atm-m ³ /mol	1.08E-02	1	1.37E-02	1
H ₄ avg: kPa-m ³ /mol	1.0906		1.3868	
COV, r [std/mean]	2.62		1.38	
COV, both replic.	_____		_____	
Observation: (1)	0.4342		0.5584	
(Peak Area) (2)	0.4529		0.5544	
(3)	0.4270		0.5459	
(4)	0.4455		0.5419	
Injection: (1)	462950		556820	
(Peak Area) (2)	457740		547960	
(3)	838600		846340	
(4)	814600		850720	

Temperature Regression Parameters:

OF POINTS = 5

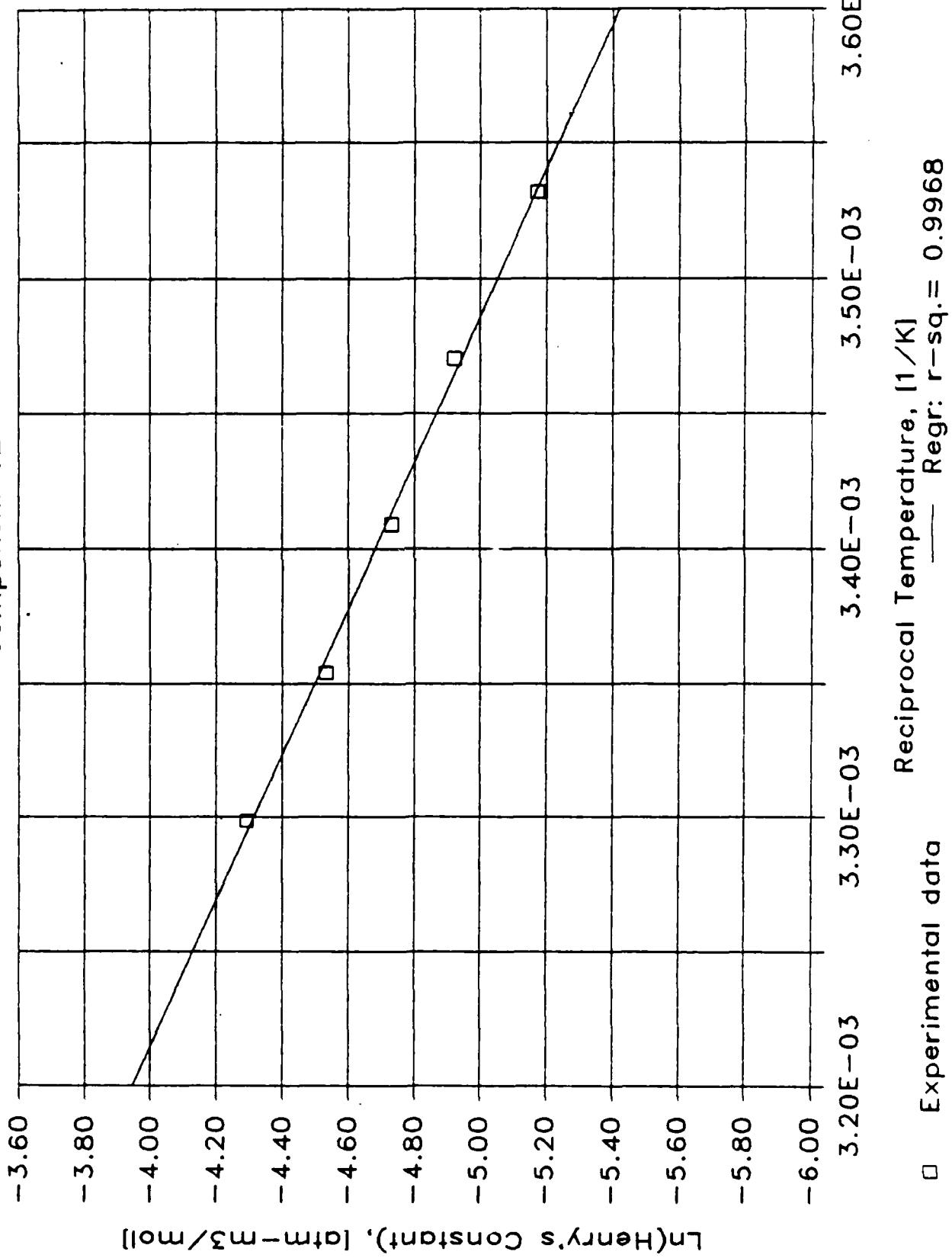
SLOPE = -3.7E+03

Y-INTERCEPT = 7.0E+00

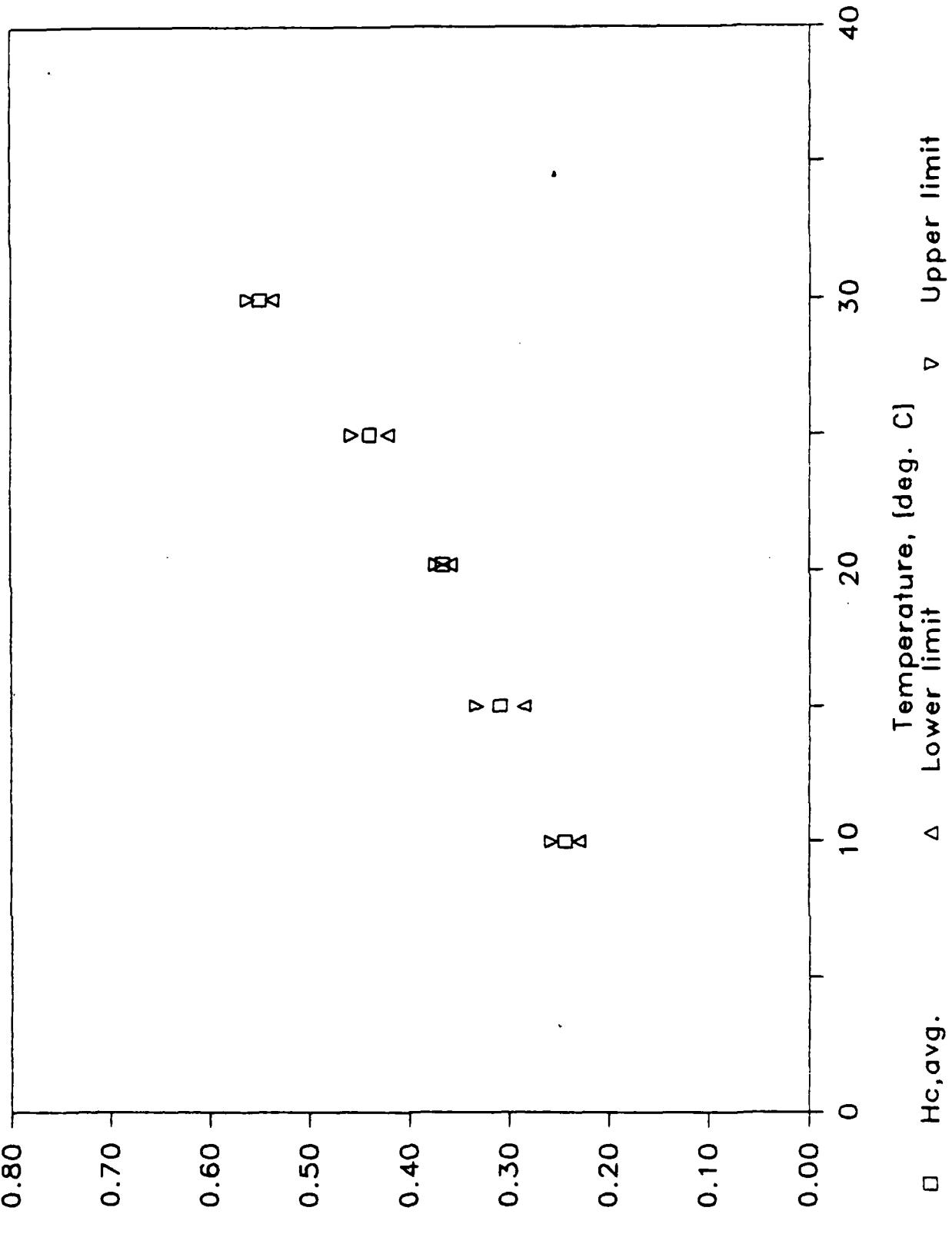
R-SQUARED = 0.9968

TEMPERATURE REGRESSION PLOT

Component 12



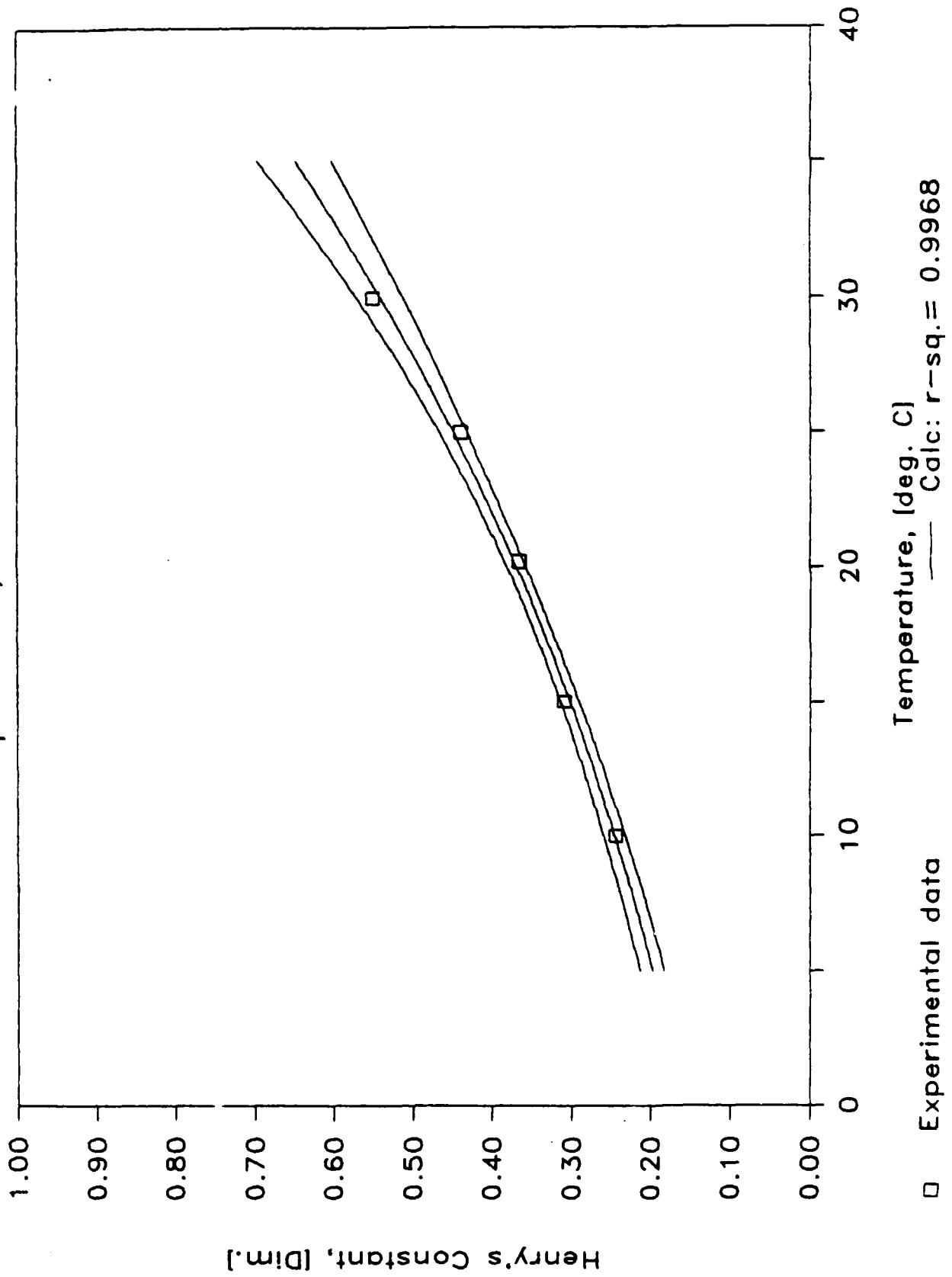
95% CONFIDENCE TEST
Component 12



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 12, 95% Confidence



86-Nov-86

Results Summary for Component 13

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	17	No. 1 No. 2	16	No. 1 No. 2	17	No. 1 No. 2
REPLICATE →						
Group No.	3		3		3	
Component ID	13		13		13	
Temperature (C)	10		15		20.2	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H _a avg: atm-m ³ /m ³	0.1982	1.0E-25	0.2764	1.0E-25	0.3054	1.0E-25
H _a avg: atm-mol/mol	245.3		362.7		408.0	
H _a avg: atm-m ³ /mol	4.42E-03	1	6.54E-03	1	7.35E-03	1
H _a avg: kPa-m ³ /mol	0.4478		0.6622		0.7448	
COV, r [std/mean]	7.48		2.97		4.71	
COV, both replic.	—		—		—	
Observation: (1)	0.2006		0.2791		0.2884	
[atm-m ³ /m ³] (2)	0.2042		0.2861		0.3009	
(3)	0.1764		0.2568		0.3094	
(4)	0.1796		0.2736		0.3226	
Injection: (1)	628740		769580		897750	
[Peak Area] (2)	586050		748450		930560	
(3)	1848900		1862200		2128100	
(4)	1830900		1833600		2071900	

96-Nov-86

Results Summary (continued)

RUN Number —>	Temperature 4		Temperature 5	
	18	23	No. 1	No. 2
REPLICATE —>				
Group No.	3		3	
Component ID	13		13	
Temperature (C)	25		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H _v avg: atm-m ³ /mol	0.3237	1.0E-25	0.4136	1.0E-25
H _v avg: atm-mol/mol	439.6		571.1	
H _v avg: atm-m ³ /mol	7.92E-03	1	1.03E-02	1
H _v avg: kPa-m ³ /mol	0.8824		1.0425	
COV, r [std/mean]	1.42		4.48	
COV, both replic.	—		—	
Observation: (1)	0.3271		0.4184	
[atm-m ³ /mol]	(2) 0.3281		0.4359	
(3) 0.3192			0.3917	
(4) 0.3292			0.4083	
Injection: (1)	1162700		1397200	
[Peak Area]	(2) 1144500		1336300	
(3) 2543700			2595700	
(4) 2538800			2524800	

Temperature Regression Parameters:

OF POINTS = 5

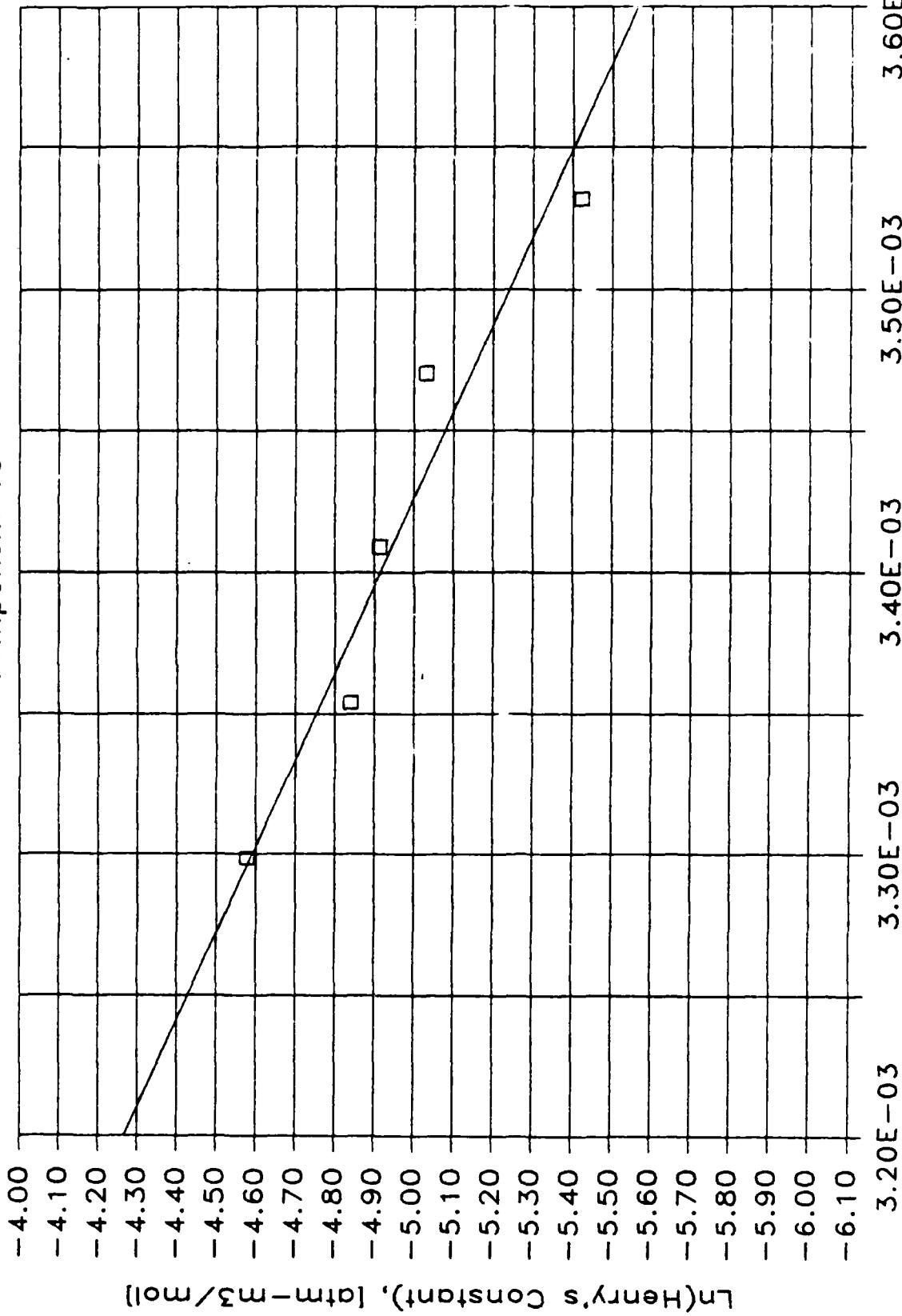
SLOPE = -3.2E+03

Y-INTERCEPT = 6.1E+08

R-SQUARED = 0.9335

TEMPERATURE REGRESSION PLOT

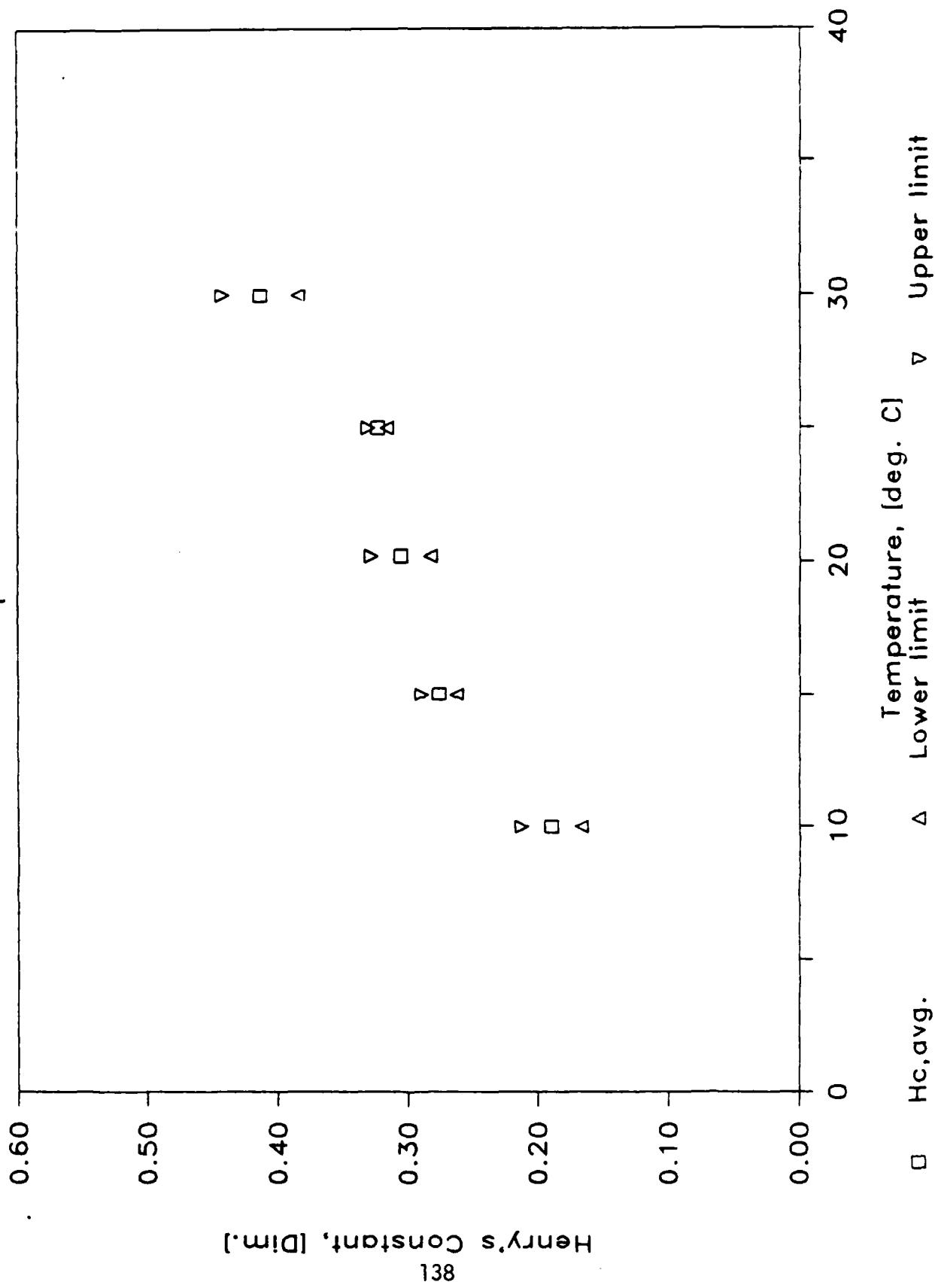
Component 13



□ Experimental data — Reciprocal Temperature, [1/K]

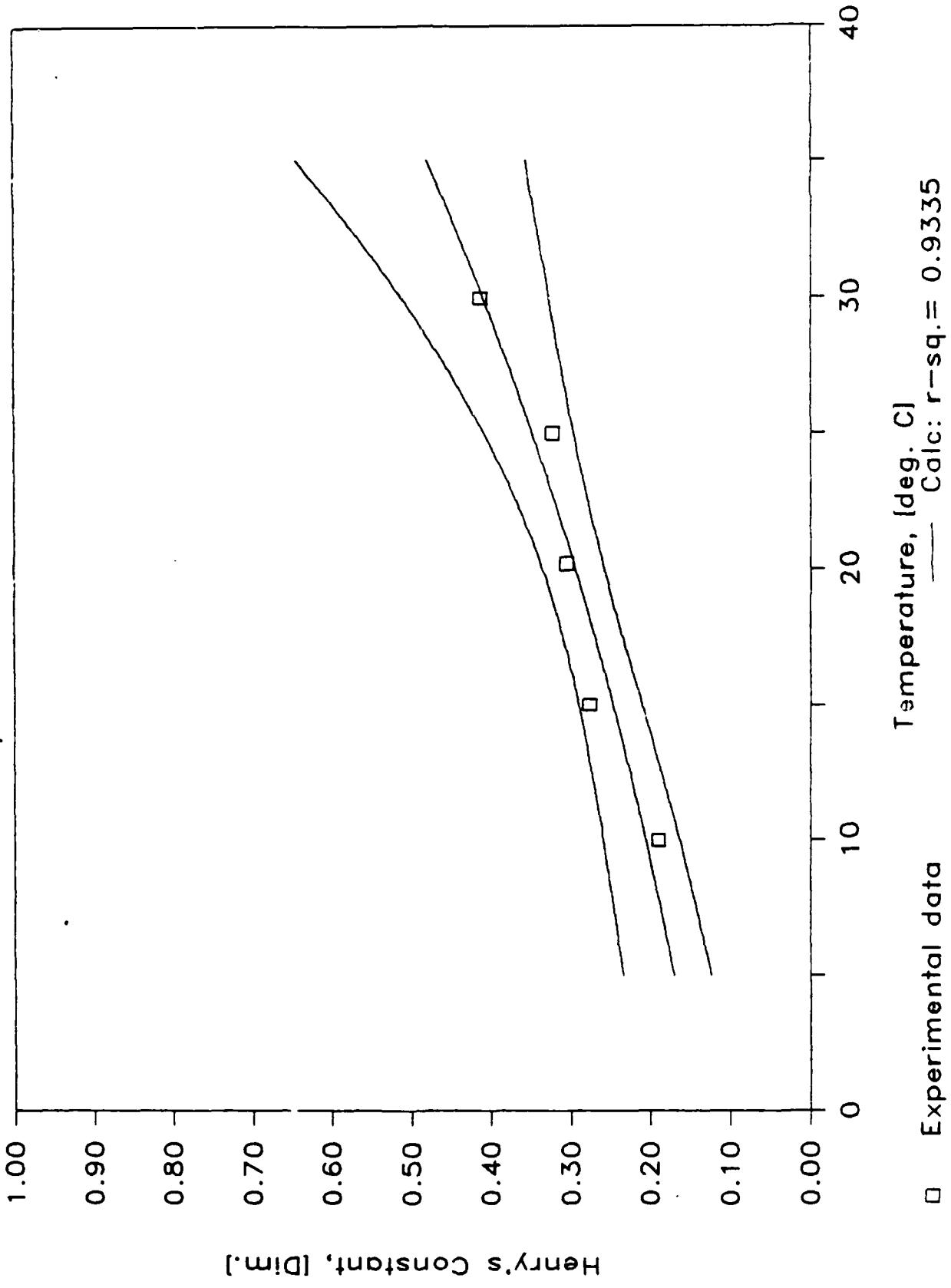
Regr: r-sq.= 0.9335

95% CONFIDENCE TEST
Component 13



REGRESSION CONFIDENCE TEST

Component 13, 95% Confidence



Henry's Constant, [Dim.]

11-Aug-86

Results Summary for Component 113

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	50	No. 1 No. 2	69	No. 1 No. 2	2	No. 1 No. 2
REPLICATE -->						
Group No.	15		15		15	
Component ID	113		113		113	
Temperature (C)	10		15.2		19.9	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H ₂ avg: atm-m3/m3	0.1403	1.0E-25	0.1906	1.0E-25	0.2499	1.0E-25
H ₂ avg: atm-mol/mol	180.9		250.3		333.5	
H ₂ avg: atm-m3/mol	3.26E-03	1	4.51E-03	1	6.01E-03	1
H ₂ avg: kPa-m3/mol	0.3303		0.4569		0.6088	
COV, r [std/mean]	0.63		5.64		3.46	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.1403		0.1860		0.2534	
[atm-m3/m3] (2)	0.1392		0.1783		0.2599	
(3)	0.1414		0.2031		0.2400	
(4)	0.1402		0.1949		0.2462	
Injection: (1)	502780		692840		993870	
[Peak Area] (2)	504550		727200		961960	
(3)	1780800		2124200		2551400	
(4)	1787700		2173100		2512900	

11-Aug-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	70	52	No. 1	No. 2
REPLICATE -->	No. 1	No. 2	No. 1	No. 2
Group No.	15		15	
Component ID	113		113	
Temperature (C)	25.15		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H _a avg: atm-m ³ /mol	0.3220	1.0E-25	0.4237	1.0E-25
H _a avg: atm-mol/mol	437.4		585.1	
H _a avg: atm-m ³ /mol	7.88E-03	1	1.05E-02	1
H _a avg: kPa-m ³ /mol	0.7986		1.0680	
COV, r [std/mean]	2.97		2.28	
COV, both replic.	_____		_____	
Observation: (1)	0.3217		0.4188	
[atm-m ³ /mol]	(2)	0.3337		0.4346
	(3)	0.3103		0.4129
	(4)	0.3221		0.4285
Injection:	(1)	1192500		1487300
[Peak Area]	(2)	1165400		1473000
	(3)	2637500		2761100
	(4)	2575300		2692400

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

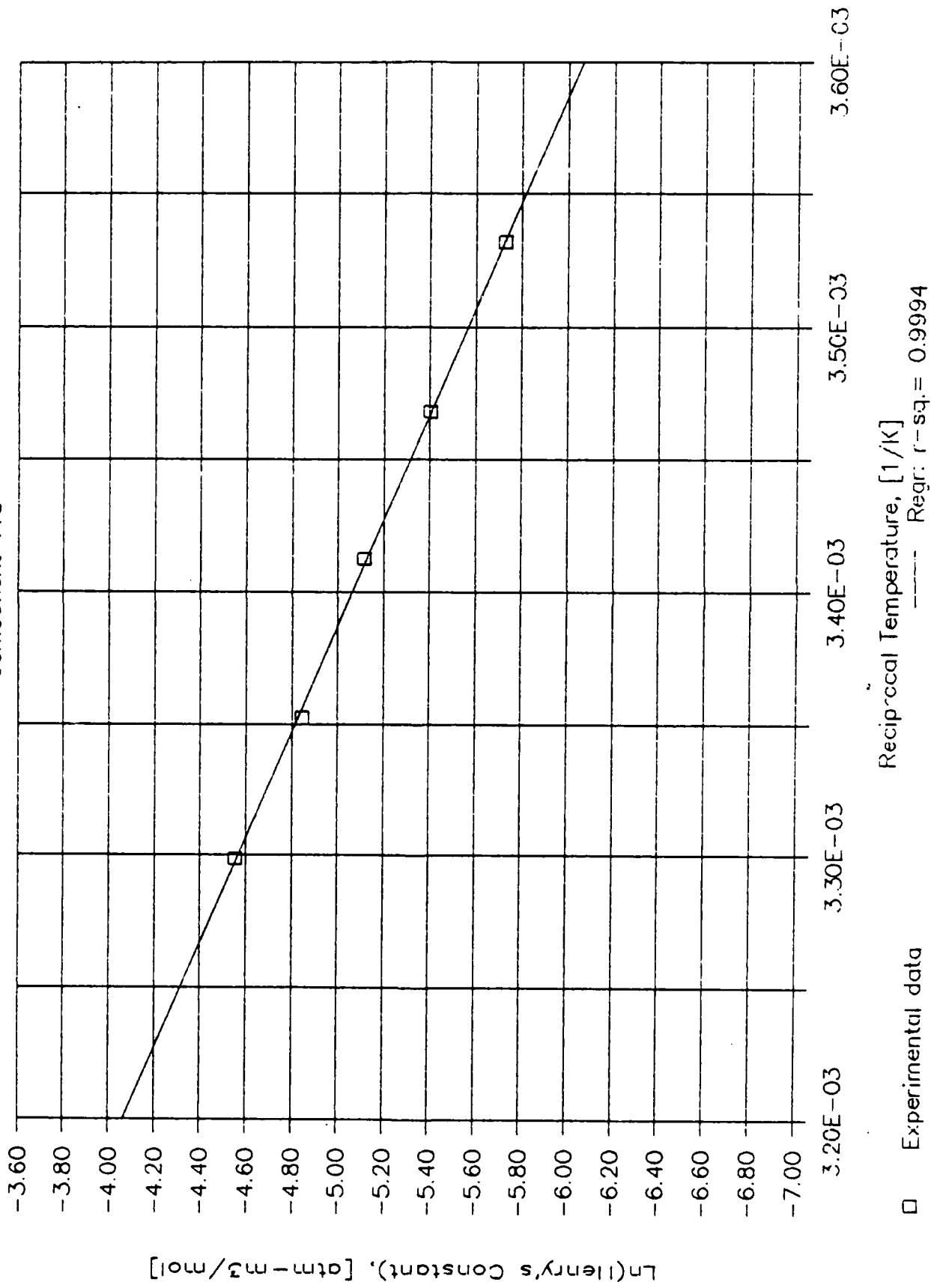
SLOPE = -5.0E+03

Y-INTERCEPT = 1.2E+01

R-SQUARED = 0.9994

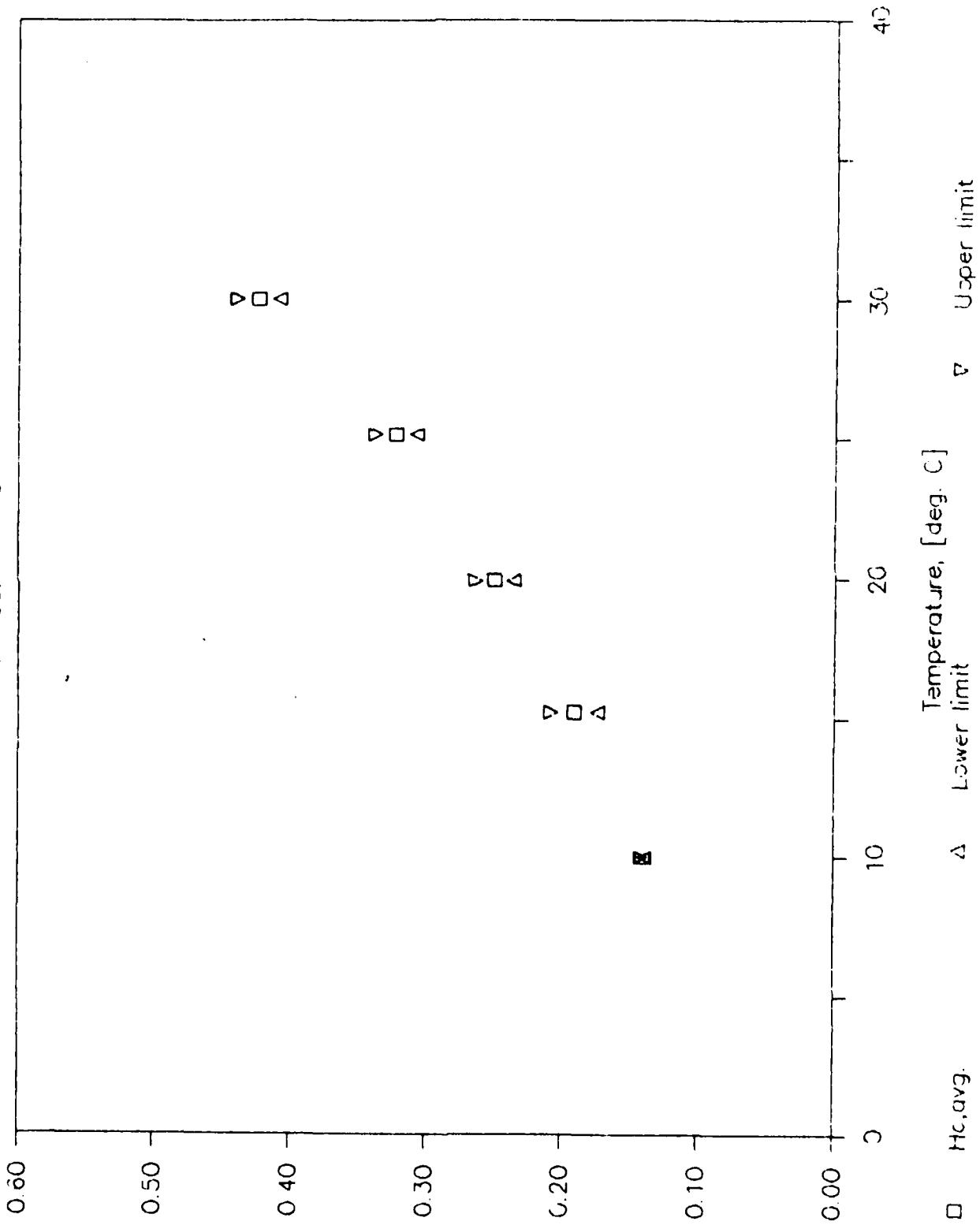
TEMPERATURE REGRESSION PLOT

Component 113



95% CONFIDENCE TEST

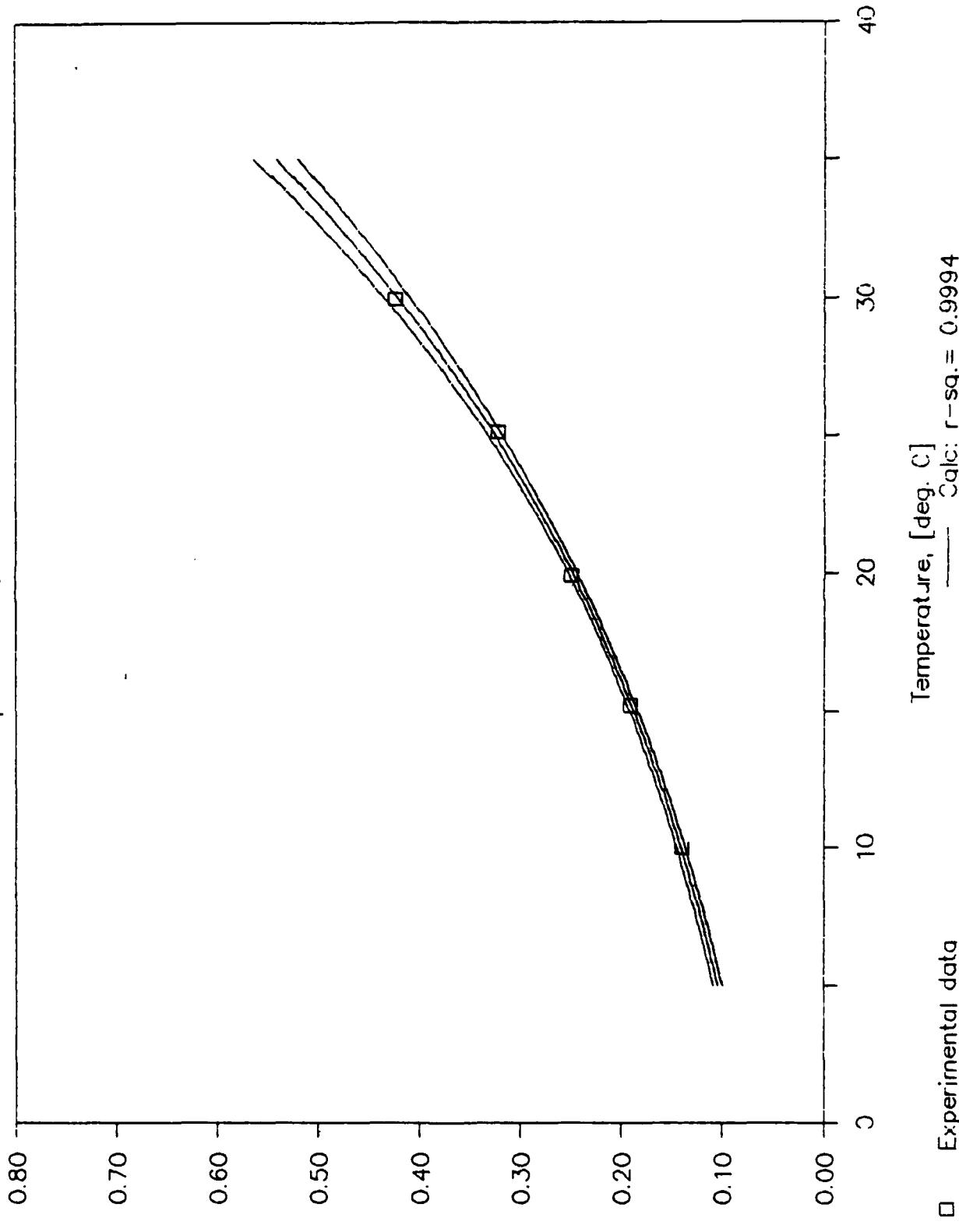
Component 113



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 113, 95% Confidence



□ Experimental data

Tempature, [deg. C]
Calc: $r - \text{sq.} = 0.9994$

06-Nov-86

Results Summary for Component 14

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	2	No. 1 No. 2	2	No. 1 No. 2	3	No. 1 No. 2
REPLICATE →						
Group No.		4		4		4
Component ID		14		14		14
Temperature (C)		10		14.9		20.1
Low Vol (ml)		25		25		25
High Vol (ml)		285		285		285
System Vol (ml)		250		250		250
H, avg: atm-m3/mol		0.1641 1.0E-25		0.2083 1.0E-25		0.2385 1.0E-25
H, avg: atm-mol/mol		211.6		273.2		307.9
H, avg: atm-m3/mol		3.81E-03	1	4.92E-03	1	5.55E-03
H, avg: kPa-m3/mol		0.3863		0.4988		0.5621
COV, r [std/mean]		5.25		7.83		2.61
COV, both replic.		_____		_____		_____
Observation: (1)		0.1626		0.2285		0.2276
[atm-m3/mol] (2)		0.1746		0.2094		0.2374
(3)		0.1537		0.2064		0.2238
(4)		0.1654		0.1887		0.2334
Injection: (1)		842930		1205500		1387400
[Peak Area] (2)		816370		1132300		1372600
(3)		2903400		3396300		3918000
(4)		2787700		3583900		3816500

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number —>		3		3	
REPLICATE —>		No. 1	No. 2	No. 1	No. 2
Group No.		4		4	
Component ID		14		14	
Temperature (C)		25		30	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H _v avg: atm-m ³ /m ³		0.2623	1.0E-25	0.3246	1.0E-25
H _v avg: atm-mol/mol		356.2		448.3	
H _v avg: atm-m ³ /mol		6.42E-03	1	8.00E-03	1
H _v avg: kPa-m ³ /mol		0.6503		0.8183	
COV, r [std/mean]		0.60		1.34	
COV, both replic.		—		—	
Observation: (1)		0.2605		0.3261	
[atm-m ³ /m ³] (2)		0.2539		0.3298	
(3)		0.2616		0.3195	
(4)		0.2641		0.3232	
Injection: (1)		1464900		2072500	
[Peak Area] (2)		1468800		2044100	
(3)		3796800		4628100	
(4)		3773200		4592800	

Temperature Regression Parameters:

OF POINTS = 5

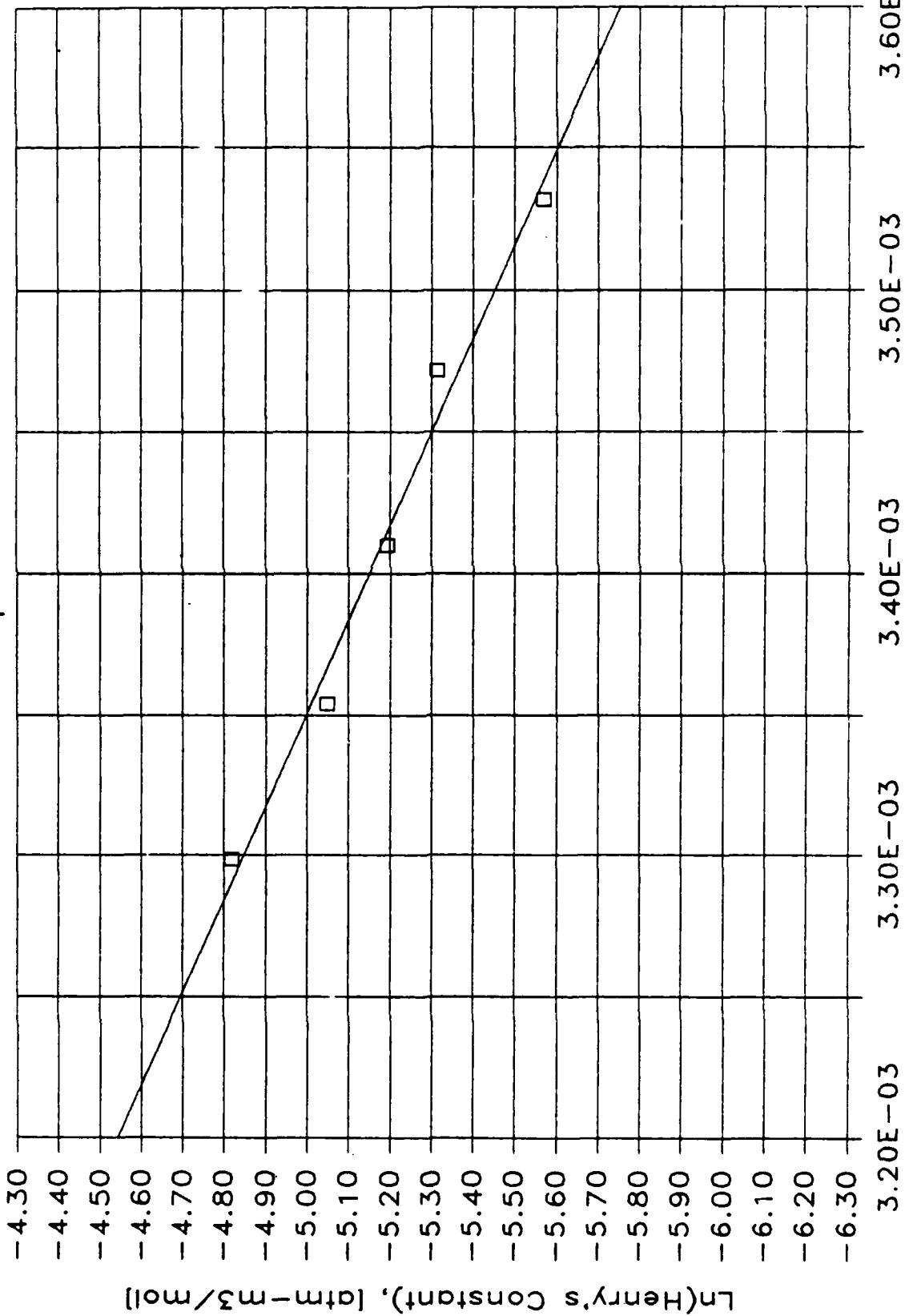
SLOPE = -3.0E+03

Y-INTERCEPT = 5.1E+00

R-SQUARED = 0.9828

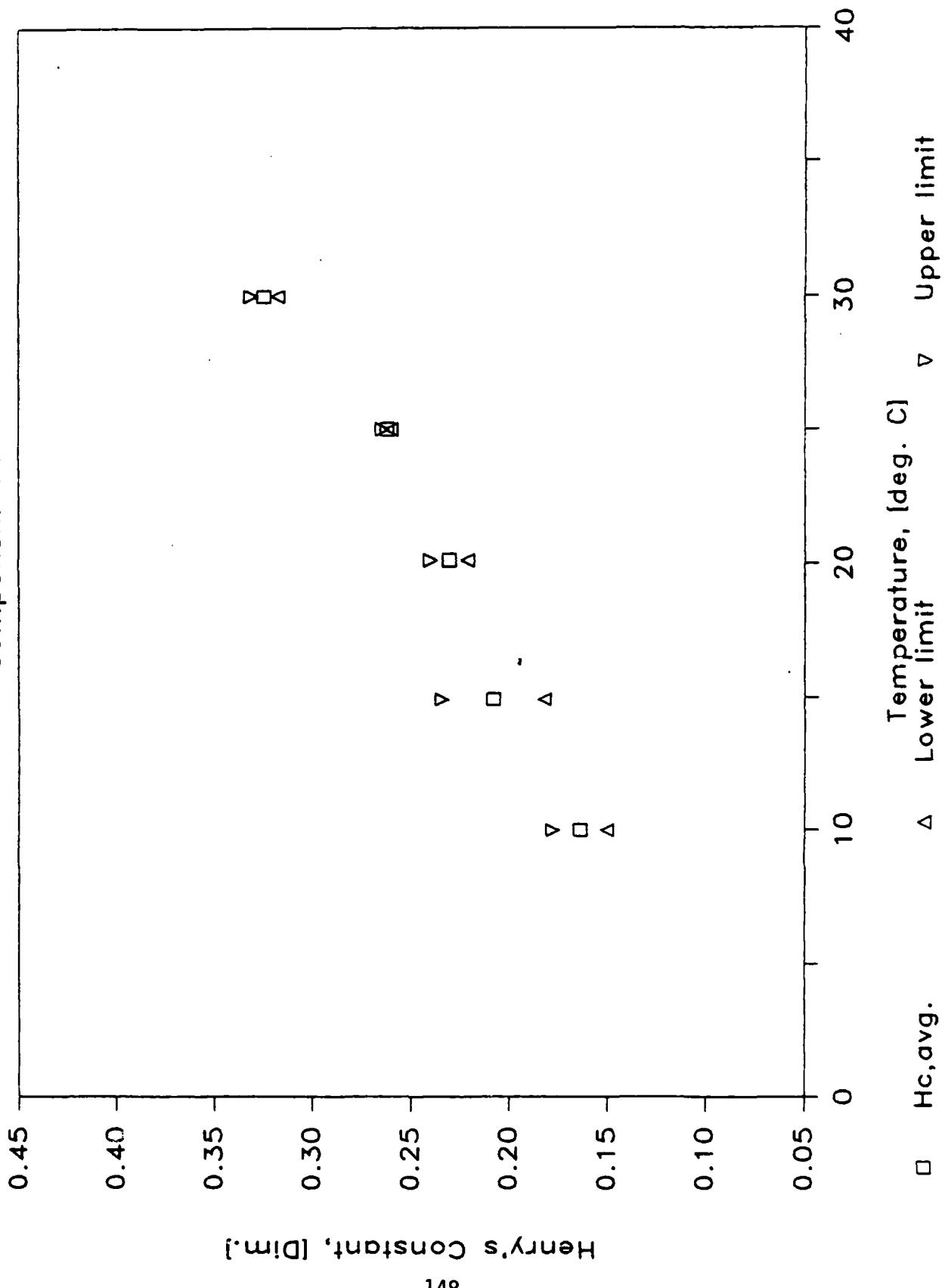
TEMPERATURE REGRESSION PLOT

Component 14



□ Experimental data Reciprocal Temperature, [1/K] Regr: r-sq. = 0.9828

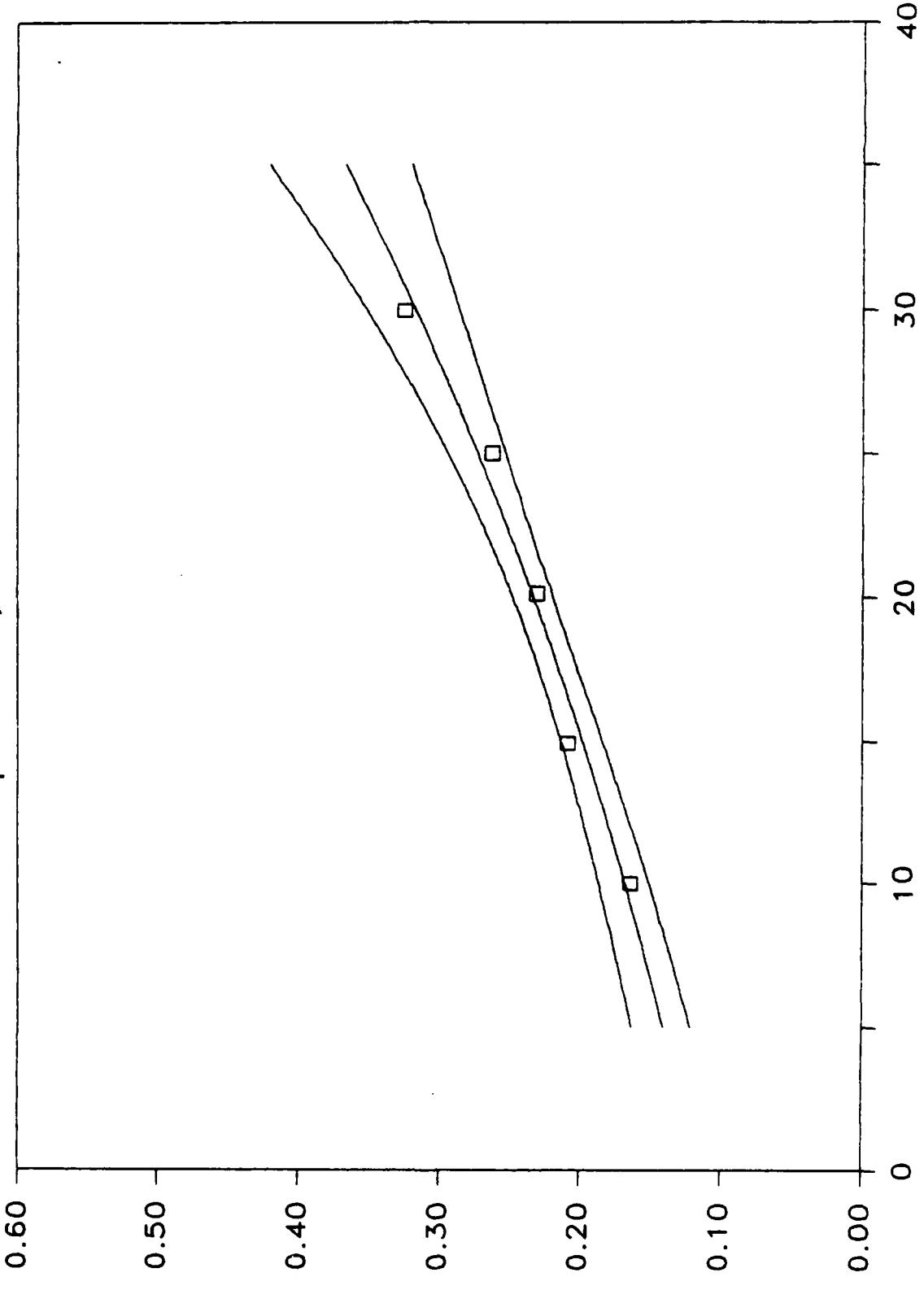
95% CONFIDENCE TEST
Component 14



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 14, 95% Confidence



□ Experimental data

— Regression line
Calcd: $r^2 = 0.9828$

06-Nov-86

Results Summary for Component 15

RUN Number →	Temperature 1		Temperature 2		Temperature 3		
	2	No. 1	2	No. 1	No. 2	No. 1	No. 2
REPLICATE →							
Group No.		9		9		9	
Component ID		15		15		15	
Temperature (C)		10		15		20	
Low Vol (ml)		21		21		21	
High Vol (ml)		201		201		201	
System Vol (ml)		250		250		250	
H _c avg: atm-m3/m3		0.1421	1.0E-25	0.1643	1.0E-25	0.1879	1.0E-25
H _c avg: atm-mol/mol		183.2		215.6		250.8	
H _c avg: atm-m3/mol		3.38E-03	1	3.88E-03	1	4.52E-03	1
H _c avg: kPa-m3/mol		0.3345		0.3936		0.4579	
COV, r [std/mean]		1.50		6.35		4.83	
COV, both replic.		—		—		—	
Observation: (1)		0.1397		0.1518		0.1933	
[atm-m3/m3] (2)		0.1431		0.1626		0.1976	
(3)		0.1418		0.1657		0.1783	
(4)		0.1445		0.1771		0.1823	
Injection: (1)		423440		532750		670050	
[Peak Area] (2)		425750		502370		637720	
(3)		1661000		2066400		2163500	
(4)		1638000		1983500		2133500	

06-Nov-86

Results Summary (continued)

RUN Number —>	Temperature 4			Temperature 5		
	3			3		
REPLICATE —>	No. 1	No. 2		No. 1	No. 2	
Group No.		9			9	
Component ID		15			15	
Temperature (C)		25			30	
Low Vol (ml)		21			21	
High Vol (ml)		201			201	
System Vol (ml)		250			250	
H, avg: atm-m3/mol	0.2156	1.0E-25		0.2895	1.0E-25	
H, avg: atm-mol/mol	292.8			399.7		
H, avg: atm-m3/mol	5.28E-03	1		7.20E-03	1	
H, avg: kPa-m3/mol	0.5345			0.7297		
COV, r [std/mean]	4.72			5.24		
COV, both replic.	—	—		—	—	
Observation: (1)	0.2229			0.2965		
(atm-m3/mol) (2)	0.2258			0.3067		
(3)	0.2056			0.2726		
(4)	0.2063			0.2821		
Injection: (1)	704030			984040		
[Peak Area] (2)	668700			928310		
(3)	2073300			2385500		
(4)	2056000			2329800		

Temperature Regression Parameters:

OF POINTS = 5

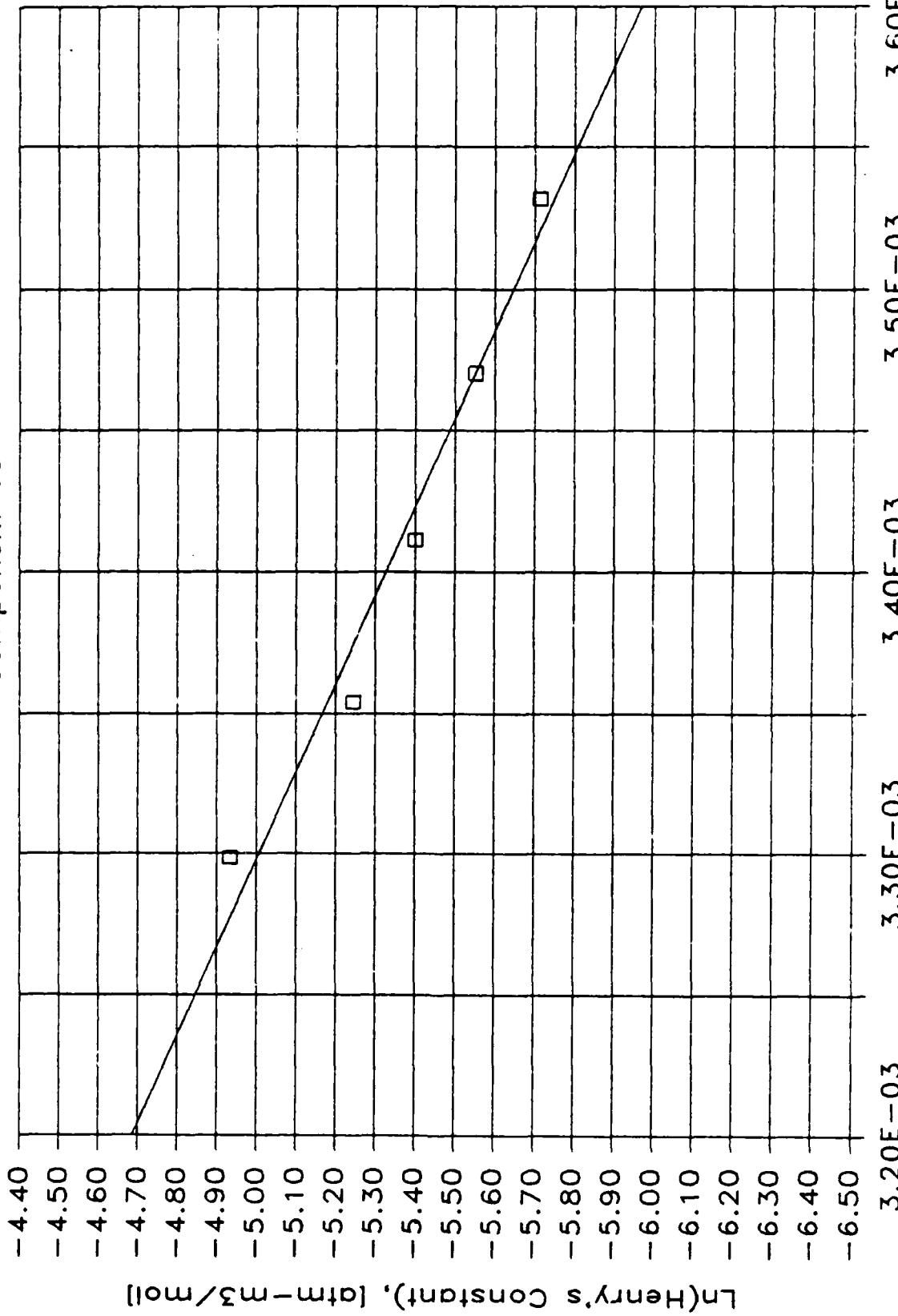
SLOPE = -3.2E+03

Y-INTERCEPT = 5.5E+00

R-SQUARED = 0.9677

TEMPERATURE REGRESSION PLOT

Component 15

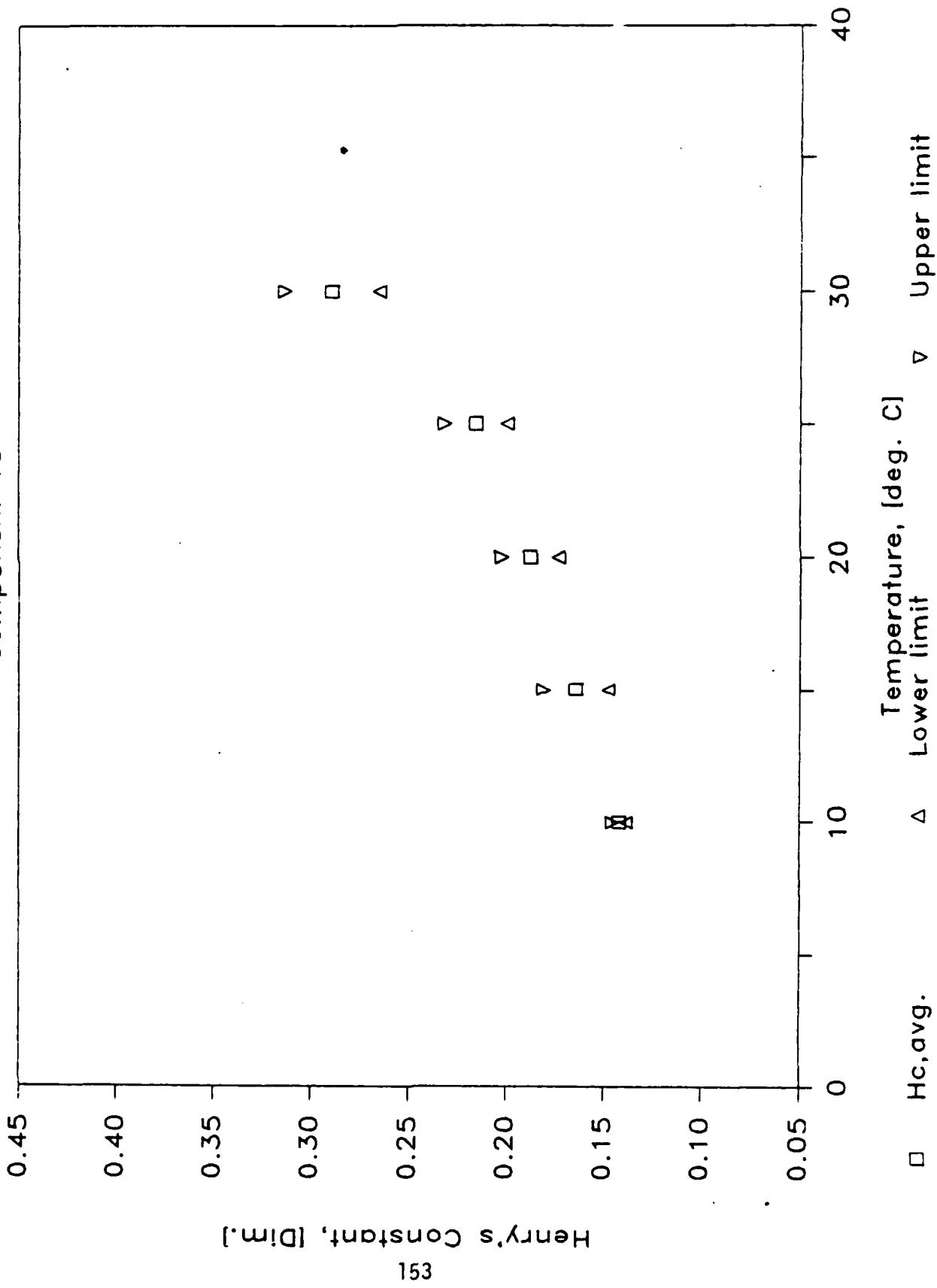


□ Experimental data

— Reciprocal Temperature, $[1/K]$
Regr: $r-sq = 0.9677$

95% CONFIDENCE TEST

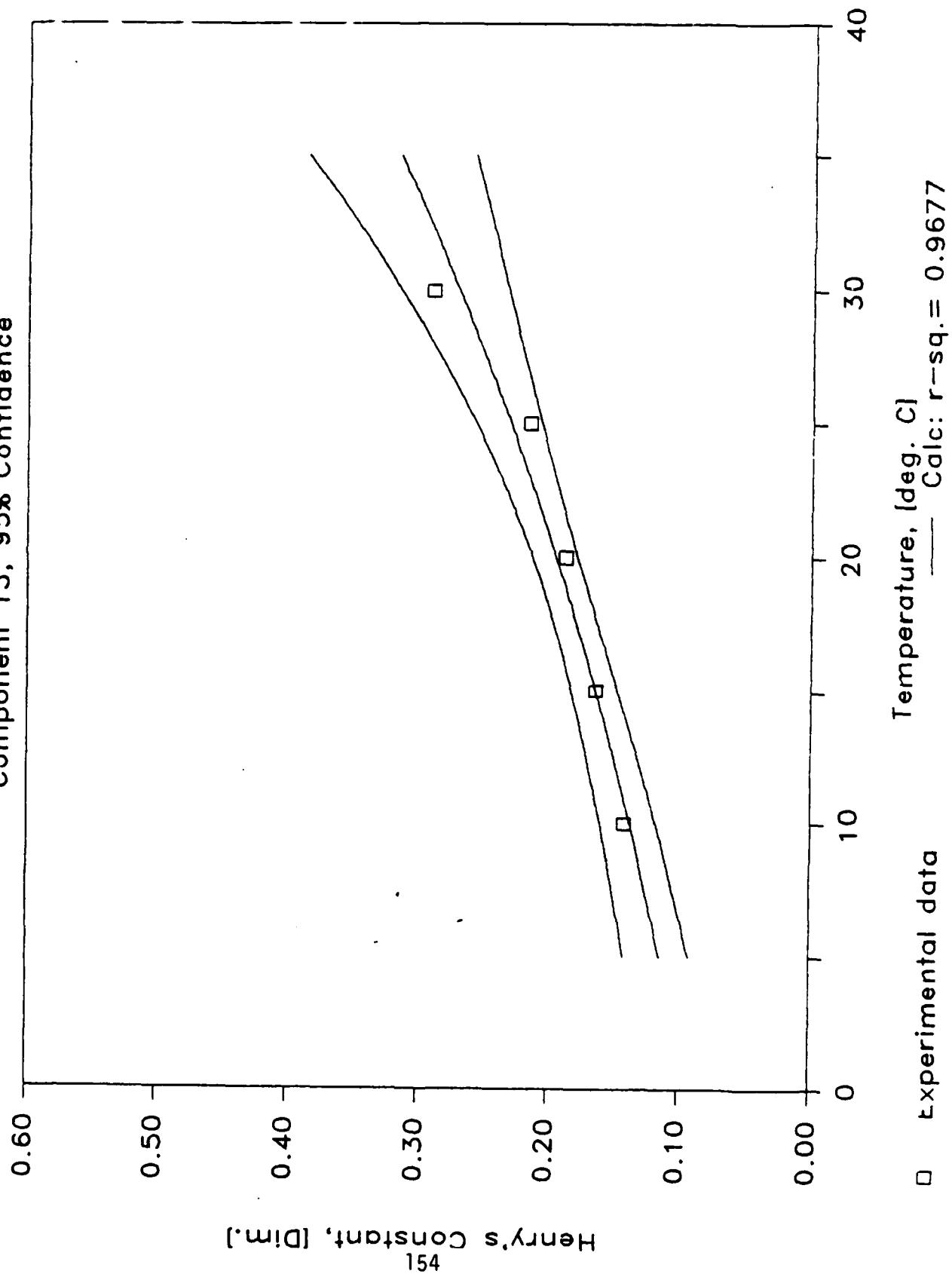
Component 15



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 15, 95% Confidence



06-Nov-86

Results Summary for Component 16

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE →						
Group No.	4		4		4	
Component ID	16		16		16	
Temperature (C)	10		14.9		20.1	
Low Vol (ml)	25		25		25	
High Vol (ml)	205		205		205	
System Vol (ml)	250		250		250	
H _c avg: atm-m ³ /m ³	0.2573	1.0E-25	0.3454	1.0E-25	0.4072	1.0E-25
H _c avg: atm-mol/mol	331.8		453.1		543.8	
H _c avg: atm-m ³ /mol	5.98E-03	1	8.16E-03	1	9.80E-03	1
H _c avg: kPa-m ³ /mol	0.6858		0.8272		0.9928	
COV, r [std/mean]	6.02		9.57		53.81	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.2758		0.3132		0.2333	
[atm-m ³ /m ³] (2)	0.2623		0.3209		0.2849	
(3)	0.2519		0.3693		0.6279	
(4)	0.2393		0.3781		0.5625	
Injection: (1)	3400		4877		4370	
[Peak Area] (2)	3206		5459		8664	
(3)	8492		11192		12154	
(4)	8774		11011		13165	

86-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4				Temperature 5	
	12		11		No. 1	No. 2
REPLICATE →	No. 1	No. 2			No. 1	No. 2
Group No.	4				4	
Component ID	16				16	
Temperature (C)	25				30	
Low Vol (ml)	25				25	
High Vol (ml)	285				285	
System Vol (ml)	250				250	
H _{avg} : atm-m ³ /m ³	0.5257	1.0E-25			0.7479	1.0E-25
H _{avg} : atm-mol/mol	713.9				1032.7	
H _{avg} : atm-m ³ /mol	1.29E-02	1			1.86E-02	1
H _{avg} : kPa-m ³ /mol	1.3032				1.8852	
COV, r [std/mean]	5.52				5.67	
COV, both replic.	—				—	
Observation: (1)	0.5611				0.8006	
[atm-m ³ /m ³] (2)	0.5319				0.7511	
(3)	0.5184				0.7429	
(4)	0.4913				0.6971	
Injection: (1)	10118				17093	
[Peak Area] (2)	9555				16186	
(3)	15403				20084	
(4)	16810				21040	

Temperature Regression Parameters:

OF POINTS = 5

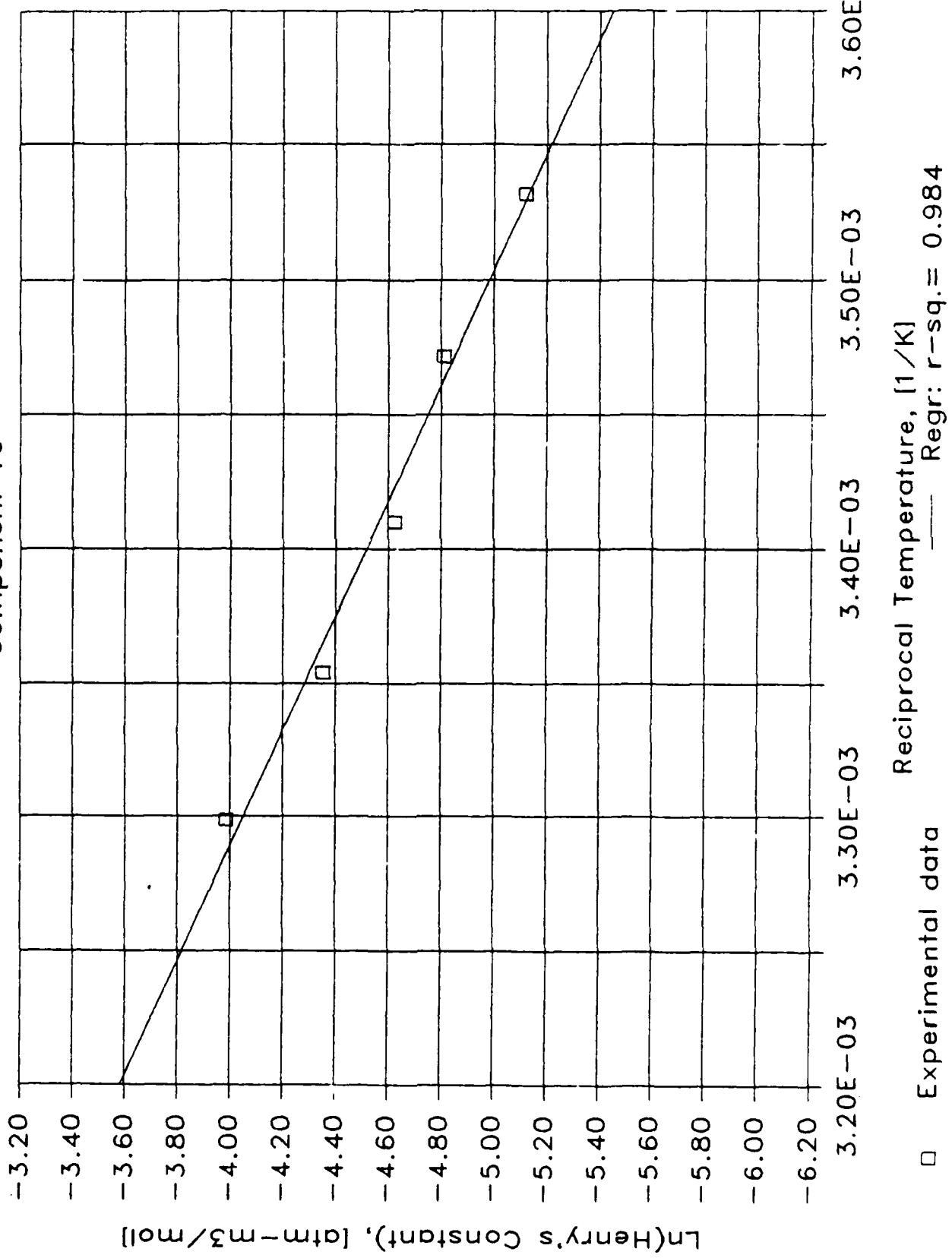
SLOPE = -4.7E+03

Y-INTERCEPT = 1.1E+01

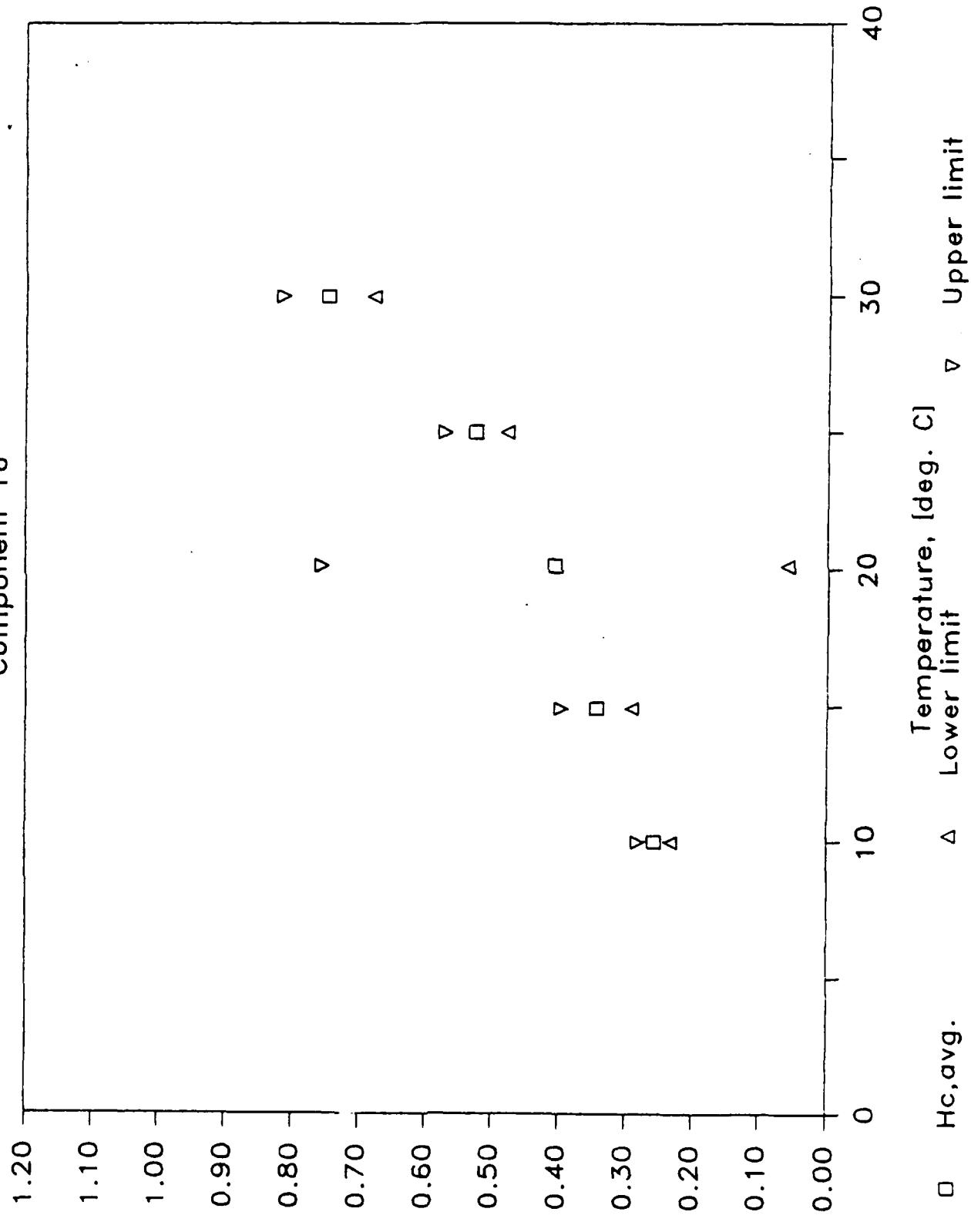
R-SQUARED = 0.9840

TEMPERATURE REGRESSION PLOT

Component 16

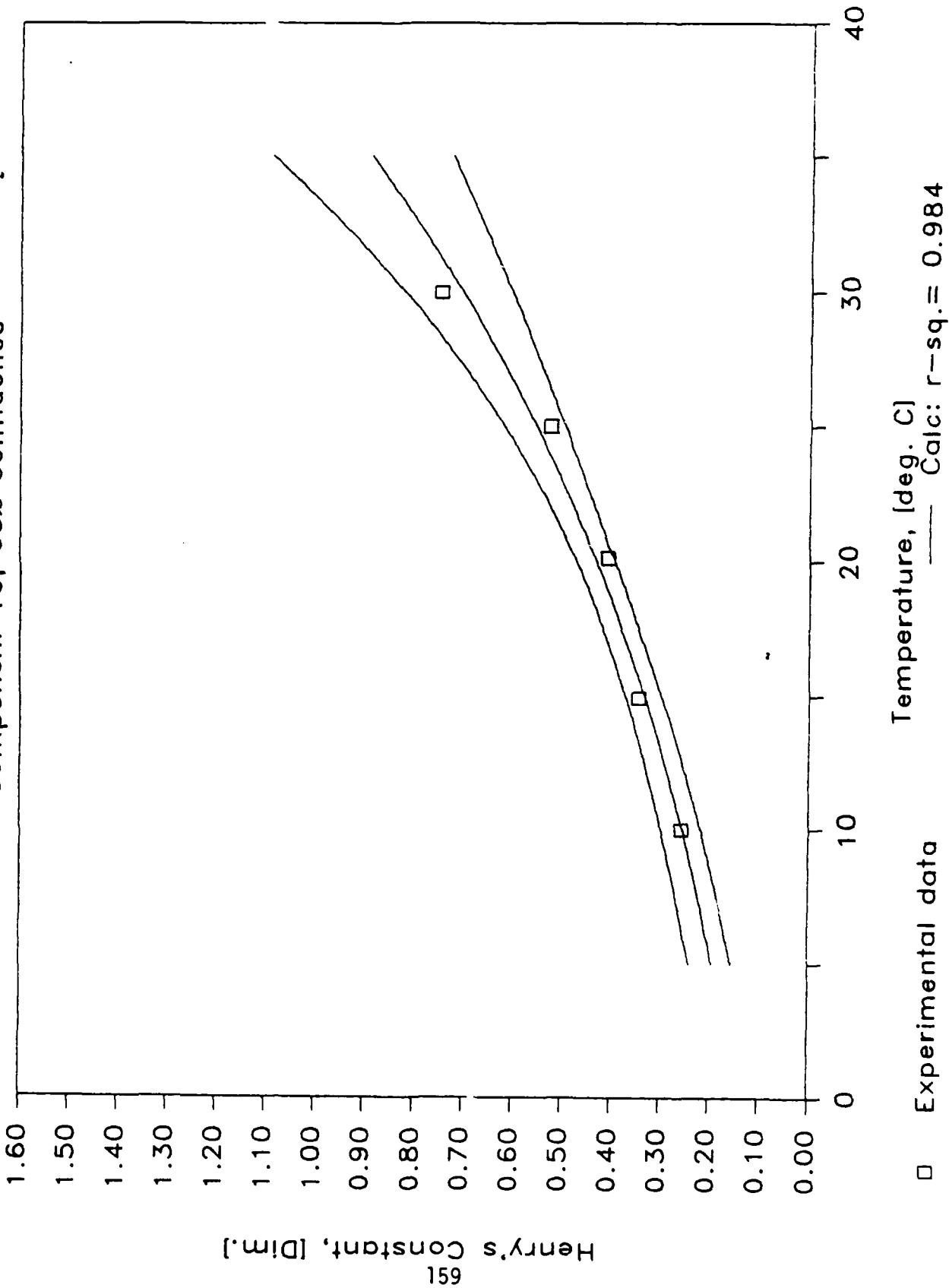


95% CONFIDENCE TEST
Component 16



REGRESSION CONFIDENCE TEST

Component 16, 95% Confidence



06-Nov-86

Results Summary for Component 17

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
REPLICATE —>	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	4		4		4	
Component ID	17		17		17	
Temperature (C)	10		14.9		20.1	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H ₄ avg: atm-m ³ /m ³	0.1509	1.0E-25	0.1776	1.0E-25	0.2092	1.0E-25
H ₄ avg: atm-mol/mol	194.6		233.0		279.4	
H ₄ avg: atm-m ³ /mol	3.51E-03	1	4.20E-03	1	5.03E-03	1
H ₄ avg: kPa-m ³ /mol	0.3552		0.4253		0.5100	
COV, r [std/mean]	1.66		2.38		3.61	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.1518		0.1827		0.2126	
[atm-m ³ /m ³] (2)	0.1538		0.1779		0.2006	
(3)	0.1480		0.1772		0.2178	
(4)	0.1499		0.1724		0.2056	
Injection: (1)	128310		205480		256860	
[Peak Area] (2)	126690		202090		260430	
(3)	437310		636850		731090	
(4)	434460		645260		755360	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		17		15	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		4		4	
Component ID		17		17	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.2281	1.0E-25	0.3897	1.0E-25
H, avg: atm-mol/mol		309.8		427.7	
H, avg: atm-m3/mol		5.58E-03	1	7.70E-03	1
H, avg: kPa-m3/mol		0.5655		0.7887	
COV, r [std/mean]		1.97		1.12	
COV, both replic.		_____	_____	_____	_____
Observation: (1)		0.2268		0.3887	
[atm-m3/mol] (2)		0.2228		0.3139	
(3)		0.2335		0.3856	
(4)		0.2294		0.3187	
Injection: (1)		259598		433800	
[Peak Area] (2)		264838		438258	
(3)		711738		983360	
(4)		719228		972920	

Temperature Regression Parameters:

OF POINTS = 5

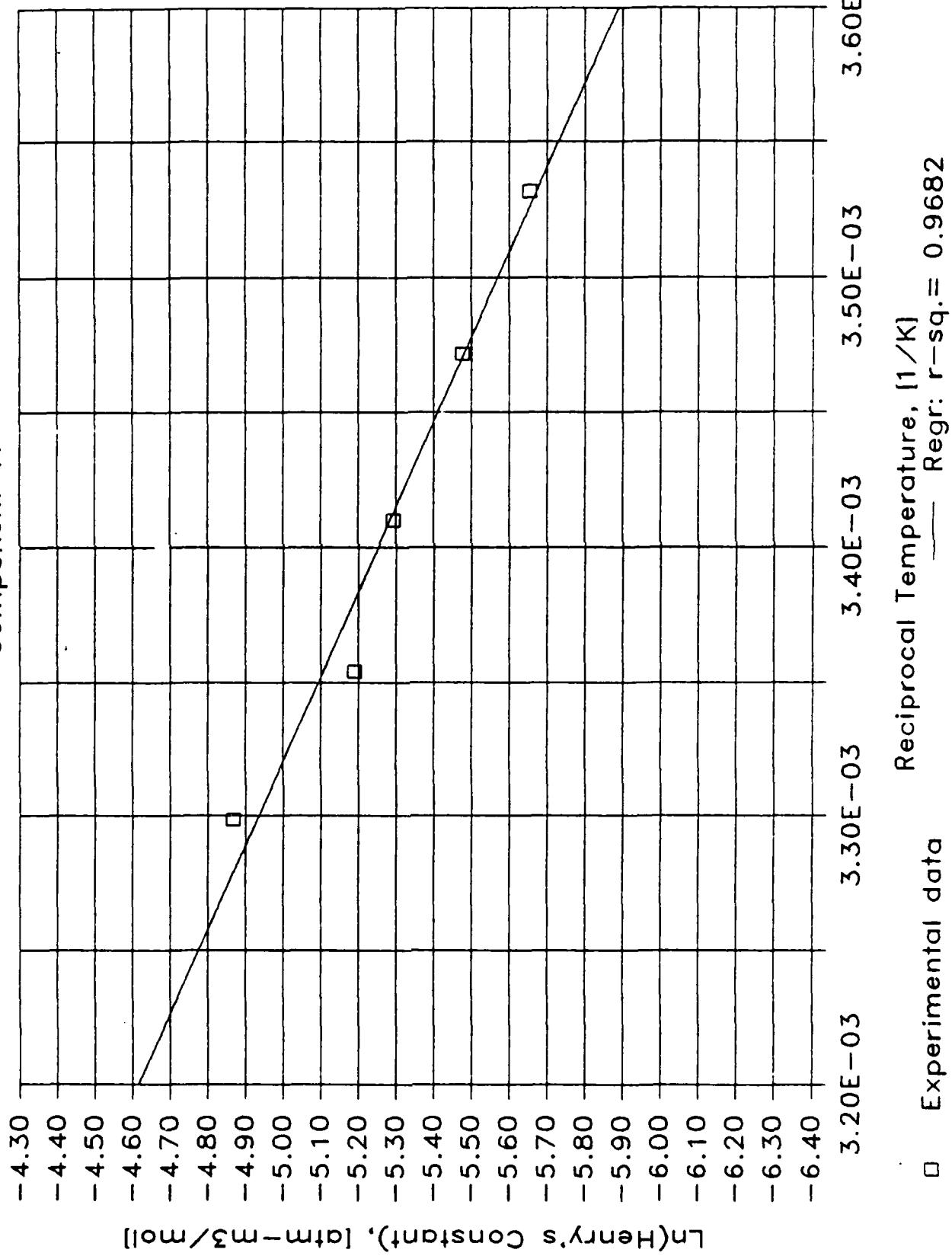
SLOPE = -3.2E+03

Y-INTERCEPT = 5.6E+00

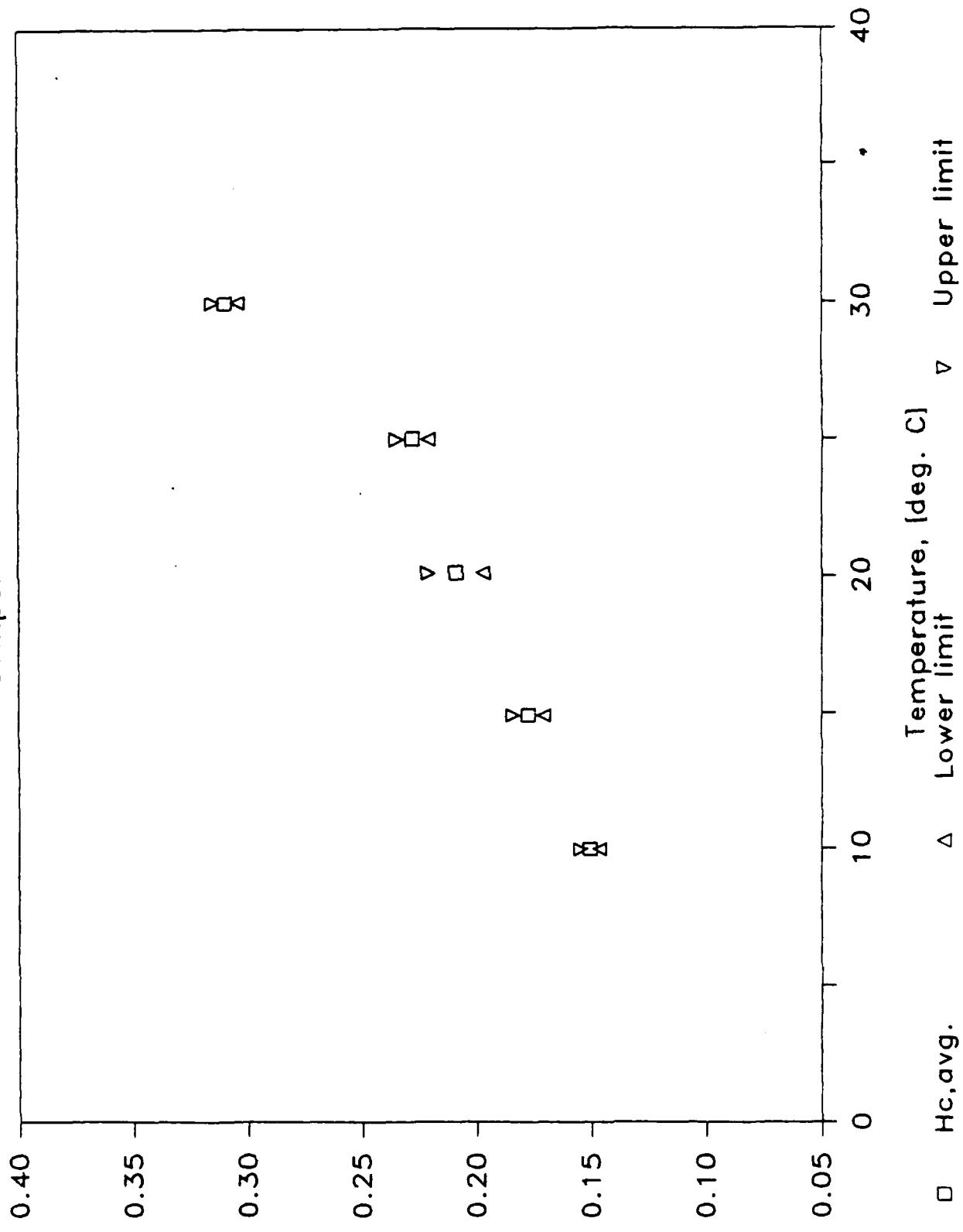
R-SQUARED = 0.9682

TEMPERATURE REGRESSION PLOT

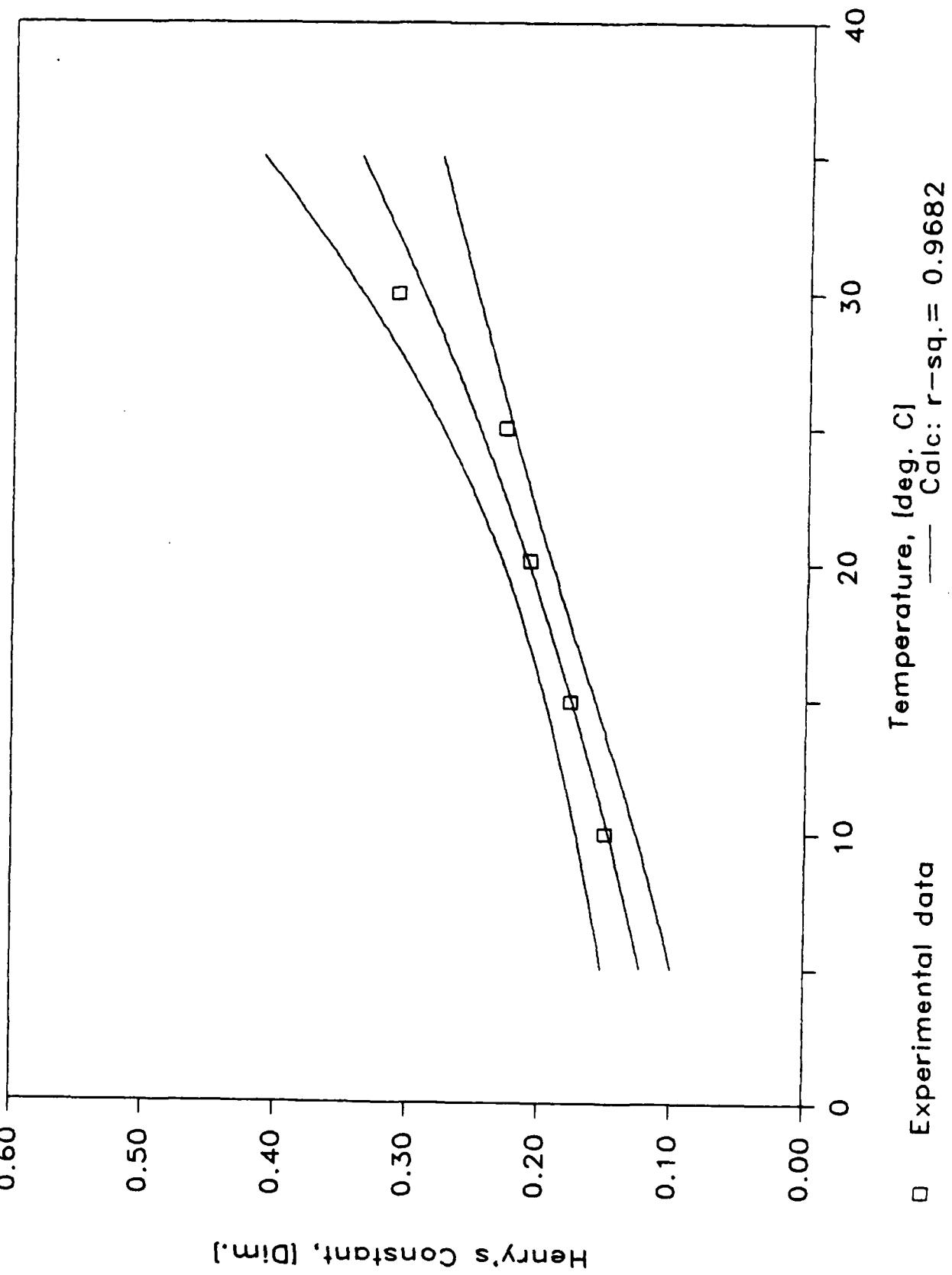
Component 17



95% CONFIDENCE TEST
Component 17



REGRESSION CONFIDENCE TEST
Component 17, 95% Confidence



86-Nov-86

Results Summary for Component 18

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
	1	2	1	2	1	2
REPLICATE —>	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	5		5		5	
Component ID	18		18		18	
Temperature (C)	10		15		20.2	
Low Vol (ml)	25		25		25	
High Vol (ml)	205		205		205	
System Vol (ml)	250		250		250	
H ₄ avg: atm-m ³ /mol	0.1583	1.0E-25	0.1920	1.0E-25	0.2340	1.0E-25
H ₄ avg: atm-mol/mol	204.1		252.1		312.7	
H ₄ avg: atm-m ³ /mol	3.68E-03	1	4.54E-03	1	5.63E-03	1
H ₄ avg: kPa-m ³ /mol	0.3726		0.4601		0.5708	
COV, r [std/mean]	2.43		2.66		1.92	
COV, both replic.	—	—	—	—	—	—
Observation: (1)	0.1630		0.1946		0.2395	
[atm-m ³ /mol] (2)	0.1588		0.1978		0.2339	
(3)	0.1577		0.1864		0.2340	
(4)	0.1536		0.1894		0.2285	
Injection: (1)	1638800		1825900		2181000	
[Peak Area] (2)	1609100		1779700		2149300	
(3)	5642600		5673700		5965300	
(4)	5724900		5619900		6054900	

-- 86-Nov-86

Results Summary (continued)

RUN Number —>	Temperature 4		Temperature 5	
	2	3	2	3
REPLICATE —>	No. 1	No. 2	No. 1	No. 2
Group No.	5		5	
Component ID	18		18	
Temperature (C)	24.9		29.9	
Low Vol (ml)	25		25	
High Vol (ml)	205		205	
System Vol (ml)	250		250	
H _{avg} : atm=m3/m3	0.2556	1.8E-25	0.3122	1.8E-25
H _{avg} :atm=mol/mol	347.0		438.9	
H _{avg} : atm=m3/mol	6.25E-03	1	7.76E-03	1
H _{avg} : kPa=m3/mol	0.6334		0.7867	
COV, r [std/mean]	1.21		2.82	
COV, both replic.	—	—	—	—
Observation: (1)	0.2598		0.3284	
[atm=m3/m3] (2)	0.2572		0.3192	
(3)	0.2548		0.3051	
(4)	0.2522		0.3040	
Injection: (1)	2788800		3695300	
[Peak Area] (2)	2753600		3576100	
(3)	7254900		8351900	
(4)	7288200		8371900	

Temperature Regression Parameters:

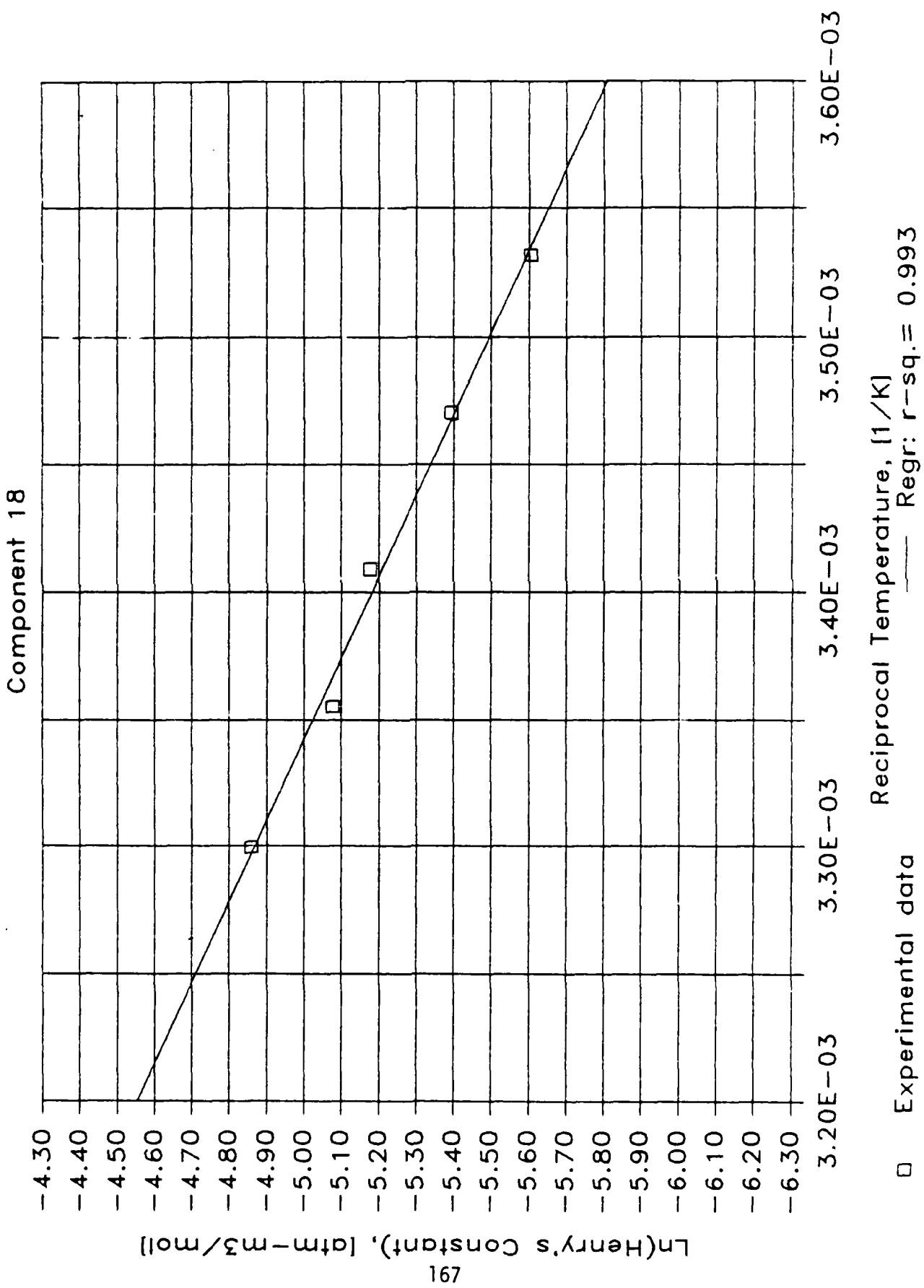
* OF POINTS = 5

SLOPE = -3.1E+03

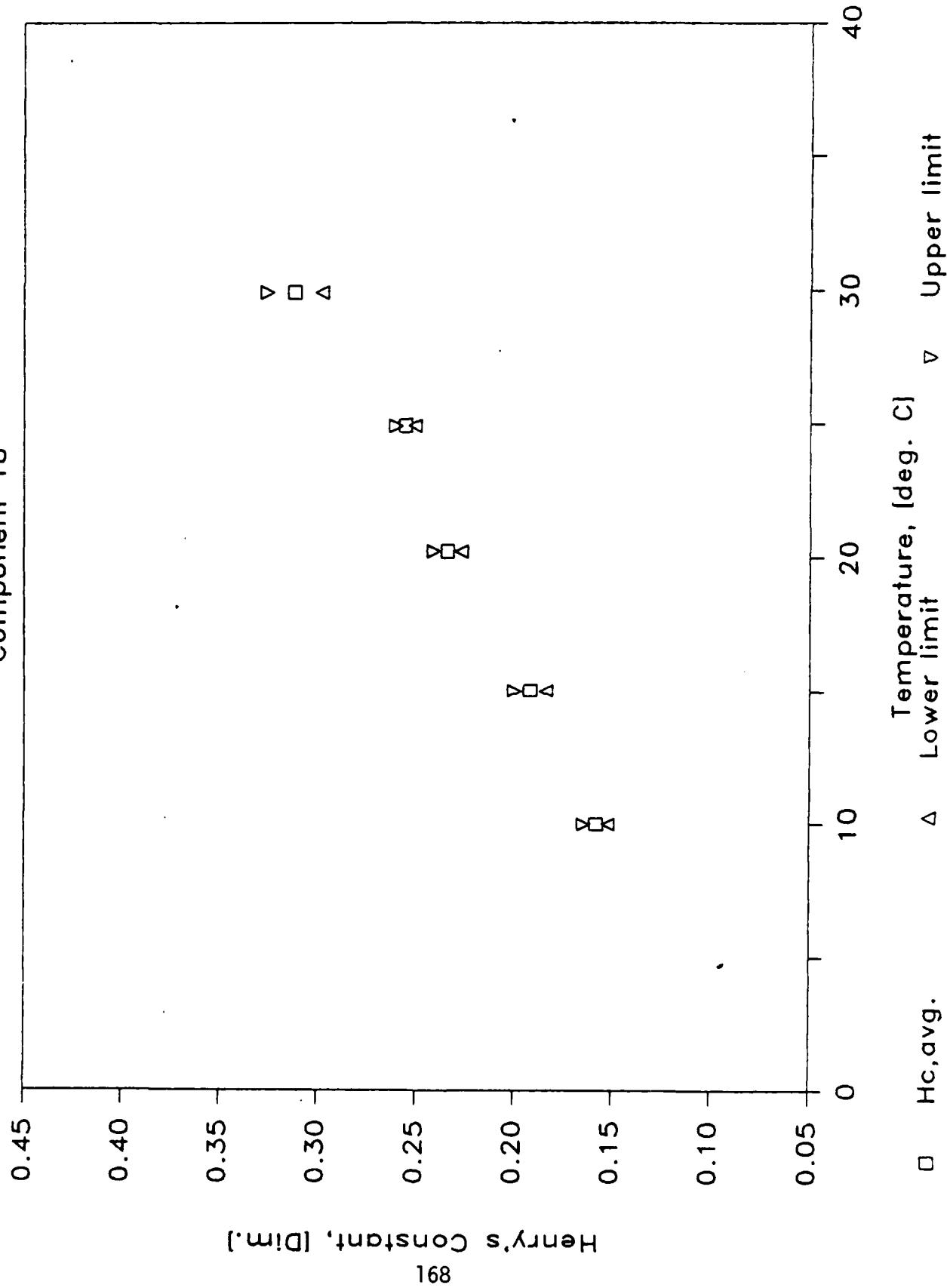
Y-INTERCEPT = 5.5E+00

R-SQUARED = 0.9930

TEMPERATURE REGRESSION PLOT

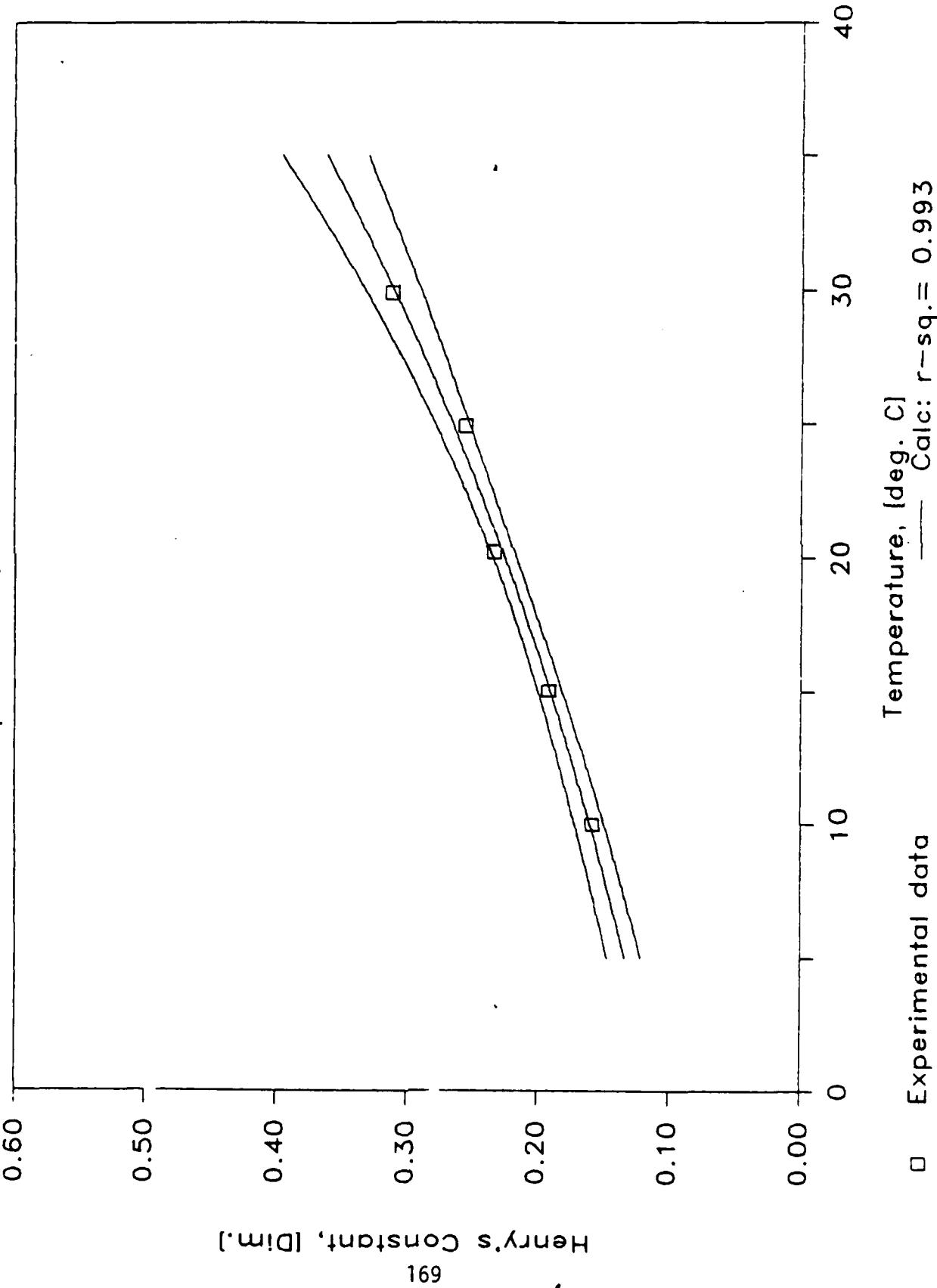


95% CONFIDENCE TEST
Component 18



REGRESSION CONFIDENCE TEST

Component 18, 95% Confidence



86-Nov-86

Results Summary for Component 19

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		5		5		6	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		5		5		5	
Component ID		19		19		19	
Temperature (C)		19		15		20.2	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H _c avg: atm-m ³ /mol		0.0503	1.0E-25	0.0549	1.0E-25	0.0612	1.0E-25
H _c avg: atm-mol/mol		64.9		72.1		81.7	
H _c avg: atm-m ³ /mol		1.17E-03	1	1.30E-03	1	1.47E-03	1
H _c avg: kPa-m ³ /mol		0.1184		0.1316		0.1492	
COV, r [std/mean]		7.49		1.23		1.91	
COV, both replic.		-----		-----		-----	
Observation: (1)		0.0526		0.0558		0.0622	
[atm-m ³ /mol] (2)		0.0543		0.0550		0.0621	
(3)		0.0463		0.0549		0.0602	
(4)		0.0480		0.0541		0.0601	
Injection: (1)		712420		880120		1087600	
(Peak Area) (2)		686070		875610		1075400	
(3)		4011000		4864500		5795100	
(4)		3971200		4886200		5798700	

06-Nov-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	6	7	6	7
REPLICATE -->	No. 1	No. 2	No. 1	No. 2
Group No.	5		5	
Component ID	19		19	
Temperature (C)	25		29.9	
Low Vol (ml)	25		25	
High Vol (ml)	205		205	
System Vol (ml)	250		250	
H, avg: atm-m3/mol	0.0577	1.0E-25	0.0701	1.0E-25
H, avg: atm-m3/mol	78.3		96.8	
H, avg: atm-m3/mol	1.41E-03	1	1.74E-03	1
H, avg: kPa-m3/mol	0.1430		0.1767	
COV, r [std/mean]	1.93		2.42	
COV, both replic.	—	—	—	—
Observation: (1)	0.0574		0.0684	
[atm-m3/mol] (2)	0.0590		0.0689	
(3)	0.0564		0.0713	
(4)	0.0580		0.0718	
Injection: (1)	1209900		1434300	
[Peak Area] (2)	1203000		1456500	
(3)	6625600		7388800	
(4)	6563600		7369000	

Temperature Regression Parameters:

OF POINTS = 5

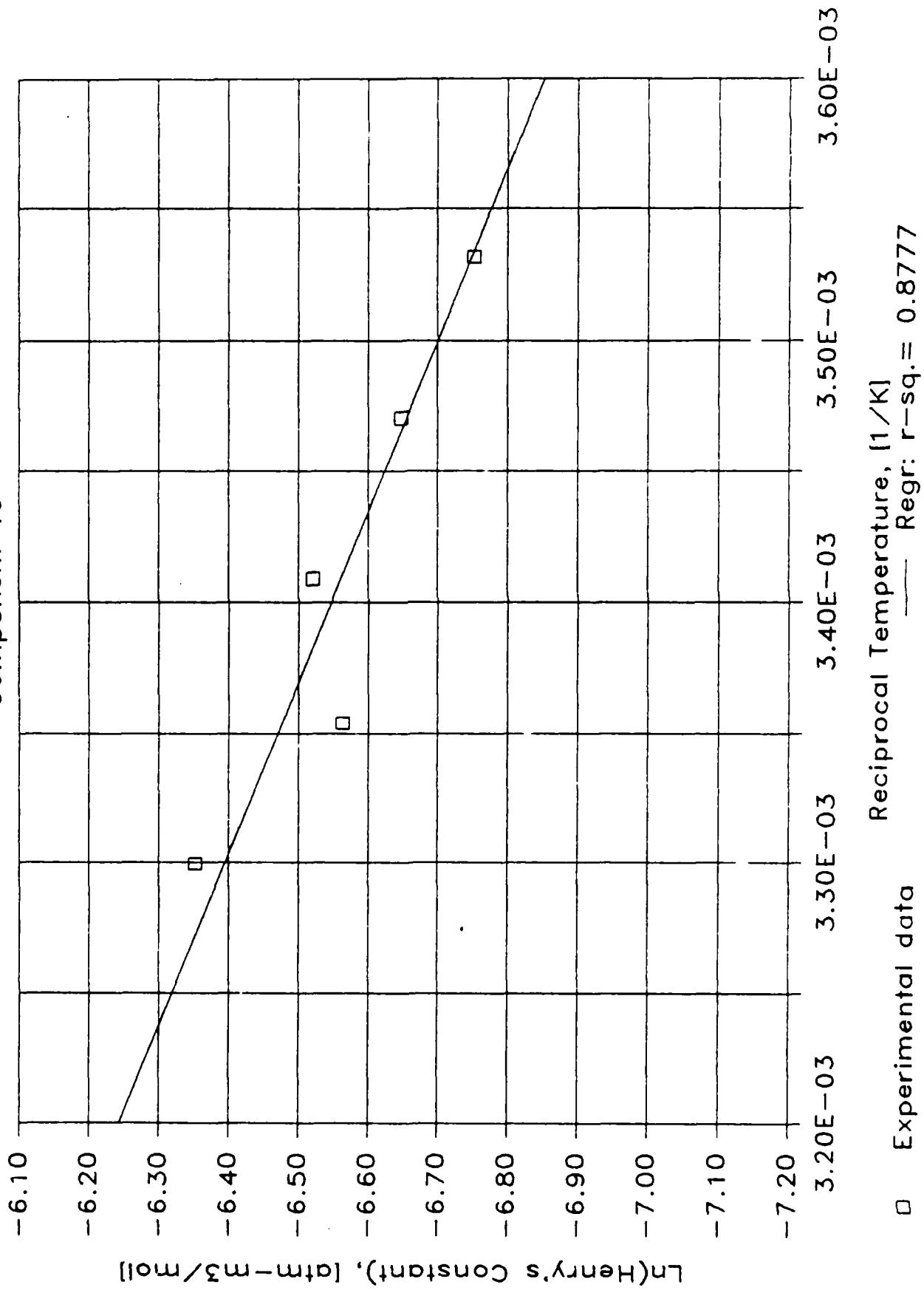
SLOPE = -1.5E+03

Y-INTERCEPT = -1.4E+00

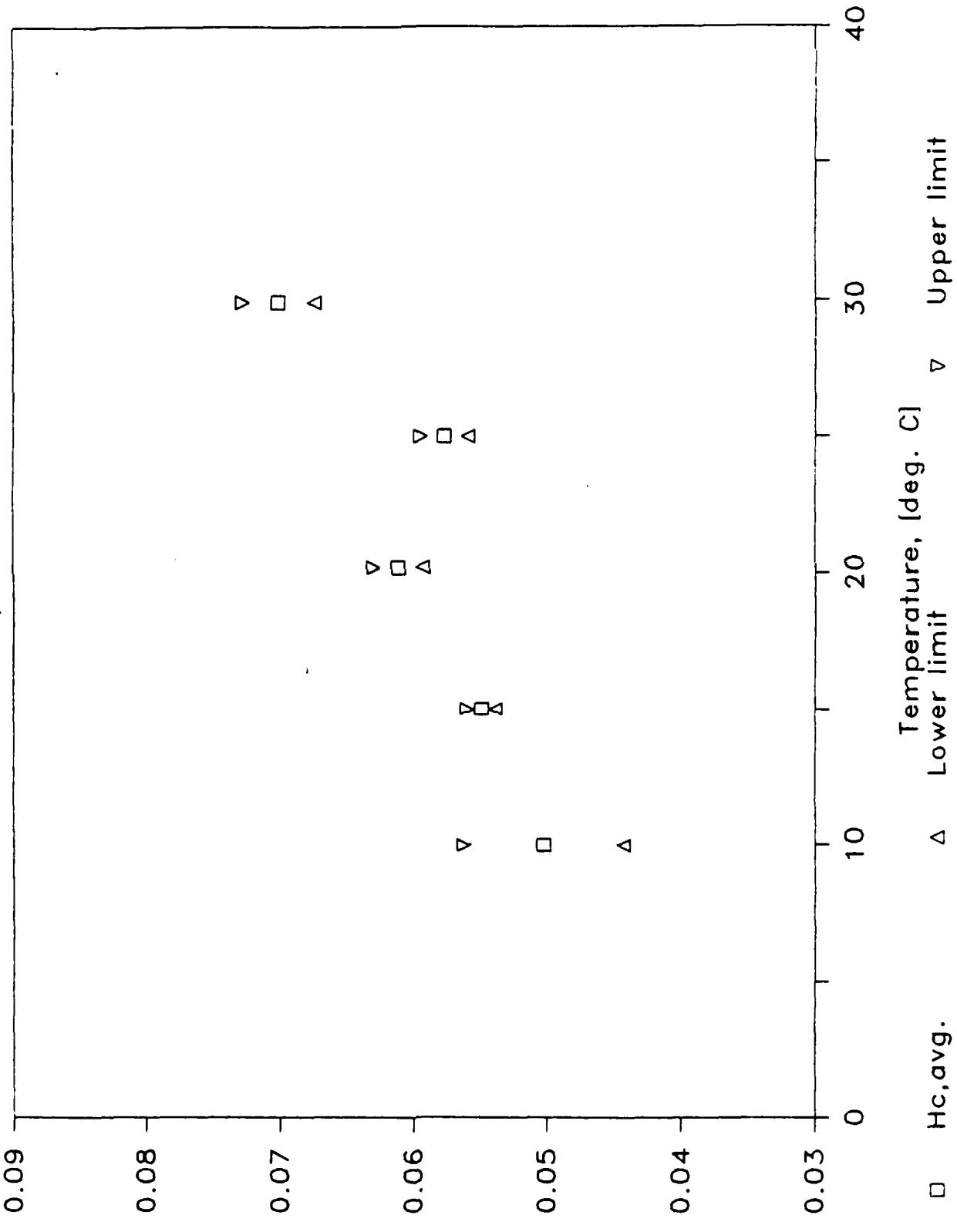
R-SQUARED = 0.8777

TEMPERATURE REGRESSION PLOT

Component 19

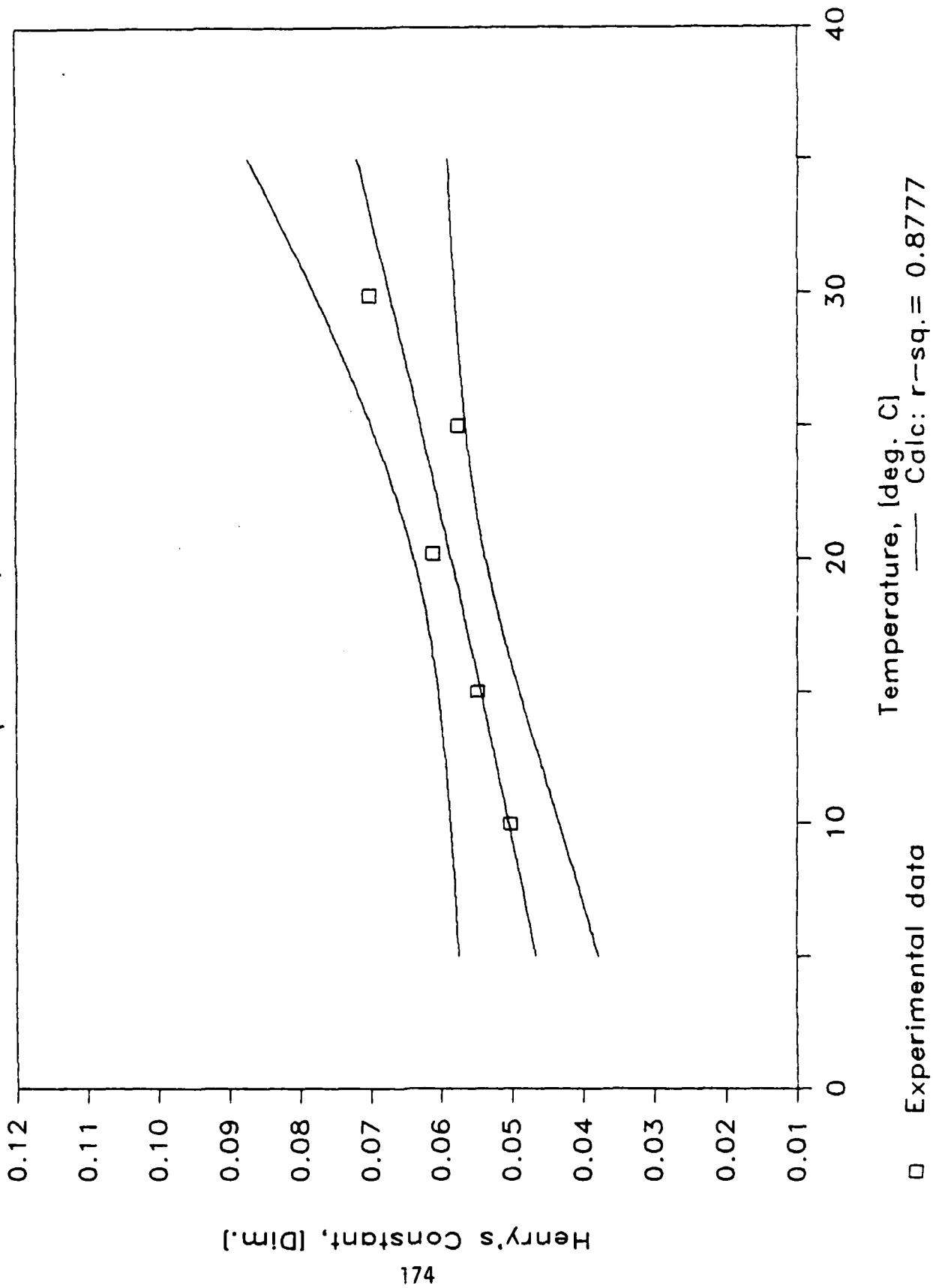


95% CONFIDENCE TEST
Component 19



REGRESSION CONFIDENCE TEST

Component 19, 95% Confidence



04-Nov-86

Results Summary for Component 119

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		48		10		6	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		1		1		1	
Component ID		19		19		19	
Temperature (C)		10.1		15		20	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H, avg: atm-m3/m3		0.0303	1.0E-25	0.0372	1.0E-25	0.0504	1.0E-25
H, avg: atm-mol/mol		39.1		48.8		67.3	
H, avg: atm-m3/mol		7.05E-04	1	8.79E-04	1	1.21E-03	1
H, avg: kPa-m3/mol		0.0714		0.0890		0.1229	
COV, r [std/mean]		4.37		4.06		7.81	
COV, both replic.		_____	_____	_____	_____	_____	_____
Observation: (1)		0.0318		0.0370		0.0530	
[atm-m3/m3] (2)		0.0310		0.0390		0.0464	
(3)		0.0296		0.0353		0.0545	
(4)		0.0289		0.0373		0.0478	
Injection: (1)		592870		769740		957000	
[Peak Area] (2)		584120		761090		965350	
(3)		3806400		4772400		5374700	
(4)		3825800		4711800		5593000	

04-Nov-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	No. 1	No. 2	No. 1	No. 2
REPLICATE -->				
Group No.	1		1	
Component ID	19		19	
Temperature (C)	25		30	
Low Vol (ml)	25		25	
High Vol (ml)	205		205	
System Vol (ml)	250		250	
H _v avg: atm-m3/m3	0.0596	1.0E-25	0.0705	1.0E-25
H _v avg: atm-mol/mol	80.9		97.3	
H _v avg: atm-m3/mol	1.46E-03	1	1.75E-03	1
H _v avg: kPa-m3/mol	0.1477		0.1777	
COV, r [std/mean]	1.57		6.87	
COV, both replic.	_____		_____	
Observation: (1) [atm-m3/m3]	0.0597		0.0702	
(2)	0.0607		0.0646	
(3)	0.0584		0.0765	
(4)	0.0594		0.0706	
Injection: (1) [Peak Area]	1222000		1432100	
(2)	1213200		1479200	
(3)	6603100		7305500	
(4)	6566300		7530500	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

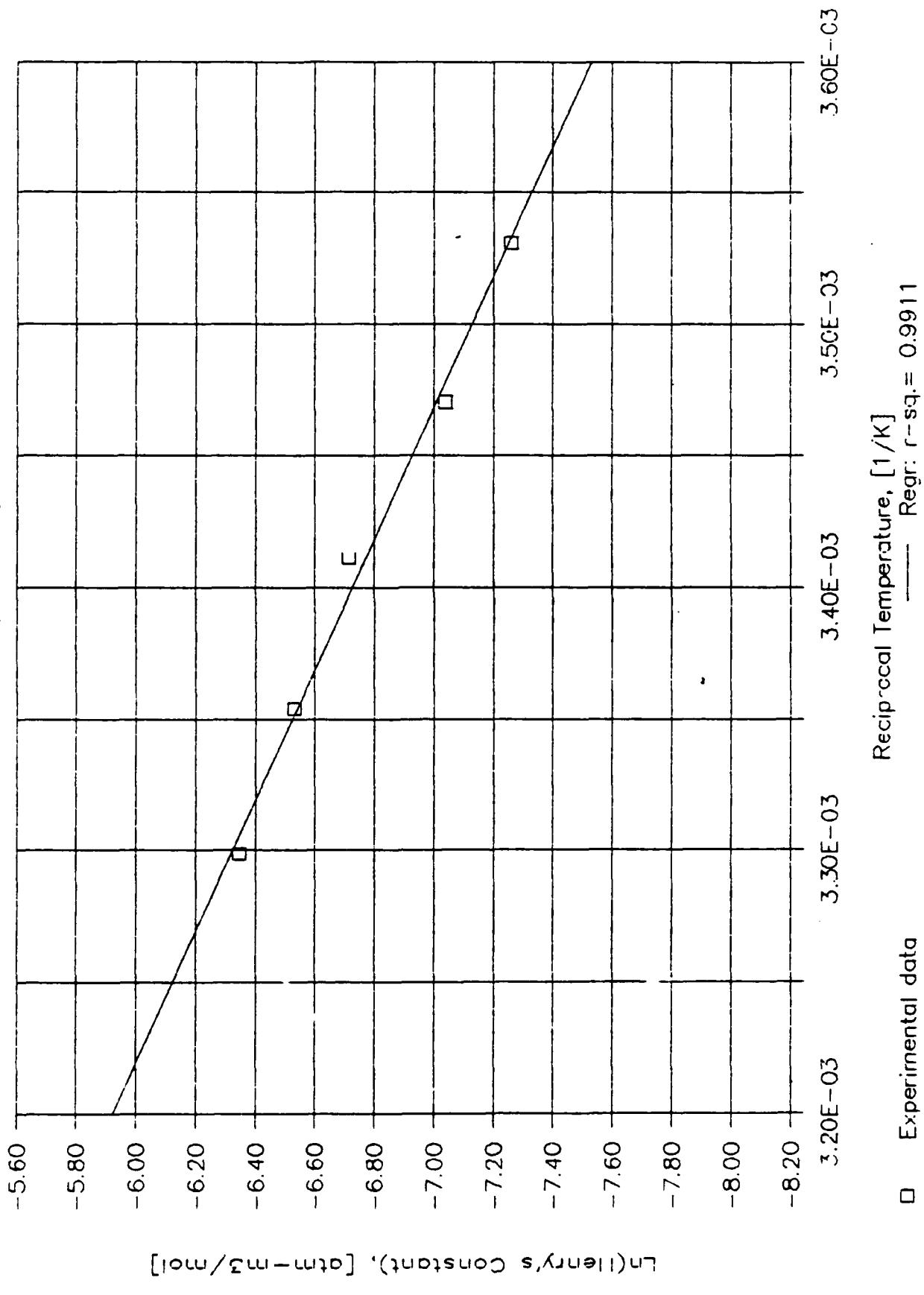
SLOPE = -4.0E+03

Y-INTERCEPT = 6.9E+00

R-SQUARED = 0.9911

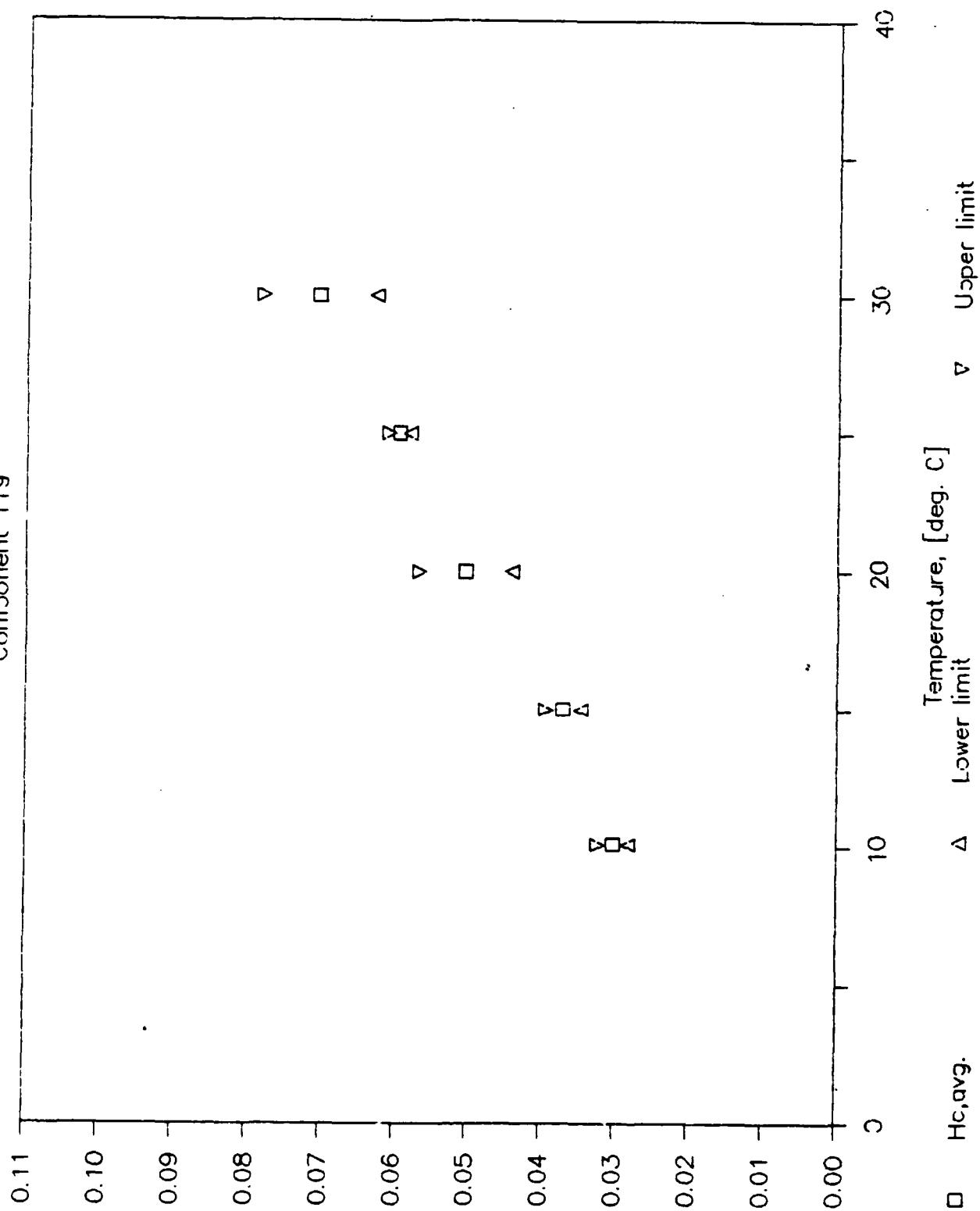
TEMPERATURE REGRESSION PLOT

Component 119



95% CONFIDENCE TEST

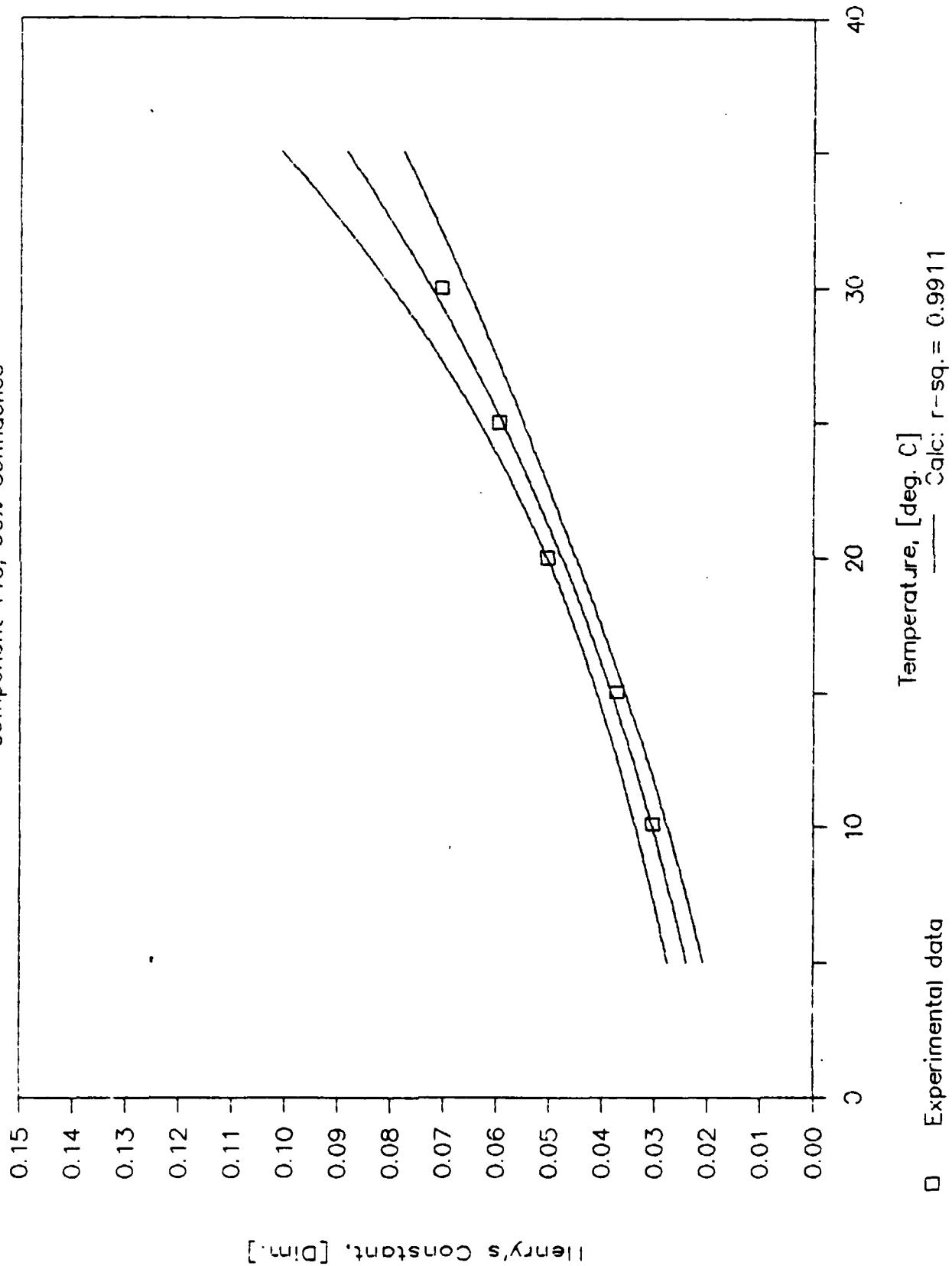
Component 119



178

REGRESSION CONFIDENCE TEST

Component 119, 95% Confidence



06-Nov-86

Results Summary for Component 20

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		9		9		10	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		5		5		5	
Component ID		20		20		20	
Temperature (C)		10		15		20.2	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H, avg: atm-m3/m3		0.4151	1.0E-25	0.4870	1.0E-25	0.6069	1.0E-25
H, avg: atm-mol/mol		535.4		639.2		810.9	
H, avg: atm-m3/mol		9.65E-03	1	1.15E-02	1	1.46E-02	1
H, avg: kPa-m3/mol		0.9774		1.1668		1.4802	
COV, r [std/mean]		2.98		5.51		0.58	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.4301		0.5012		0.5825	
[atm-m3/m3] (2)		0.4117		0.5168		0.6071	
(3)		0.4183		0.4578		0.5066	
(4)		0.4005		0.4722		0.6112	
Injection: (1)		701970		729790		871160	
[Peak Area] (2)		688380		683970		875420	
(3)		1293400		1205400		1259300	
(4)		1333800		1179100		1252400	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number —>		10		11	
REPLICATE —>		No. 1	No. 2	No. 1	No. 2
Group No.		5		5	
Component ID		20		20	
Temperature (C)		25.1		29.9	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H, avg: atm=m3/m3		0.7105	1.0E-25	0.8480	1.0E-25
H, avg: atm=mol/mol		965.2		1170.5	
H, avg: .atm=m3/mol		1.74E-02	1	2.11E-02	1
H, avg: kPa=m3/mol		1.7620		2.1367	
COV, r [std/mean]		1.35		2.24	
COV, both replic.		—	—	—	—
Observation: (1)		0.7193		0.8713	
[atm=m3/m3] (2)		0.7028		0.8463	
(3)		0.7183		0.8493	
(4)		0.7017		0.8249	
Injection: (1)		1193200		1550900	
[Peak Area] (2)		1191900		1522300	
(3)		1515800		1713400	
(4)		1541800		1750100	

Temperature Regression Parameters:

OF POINTS = 5

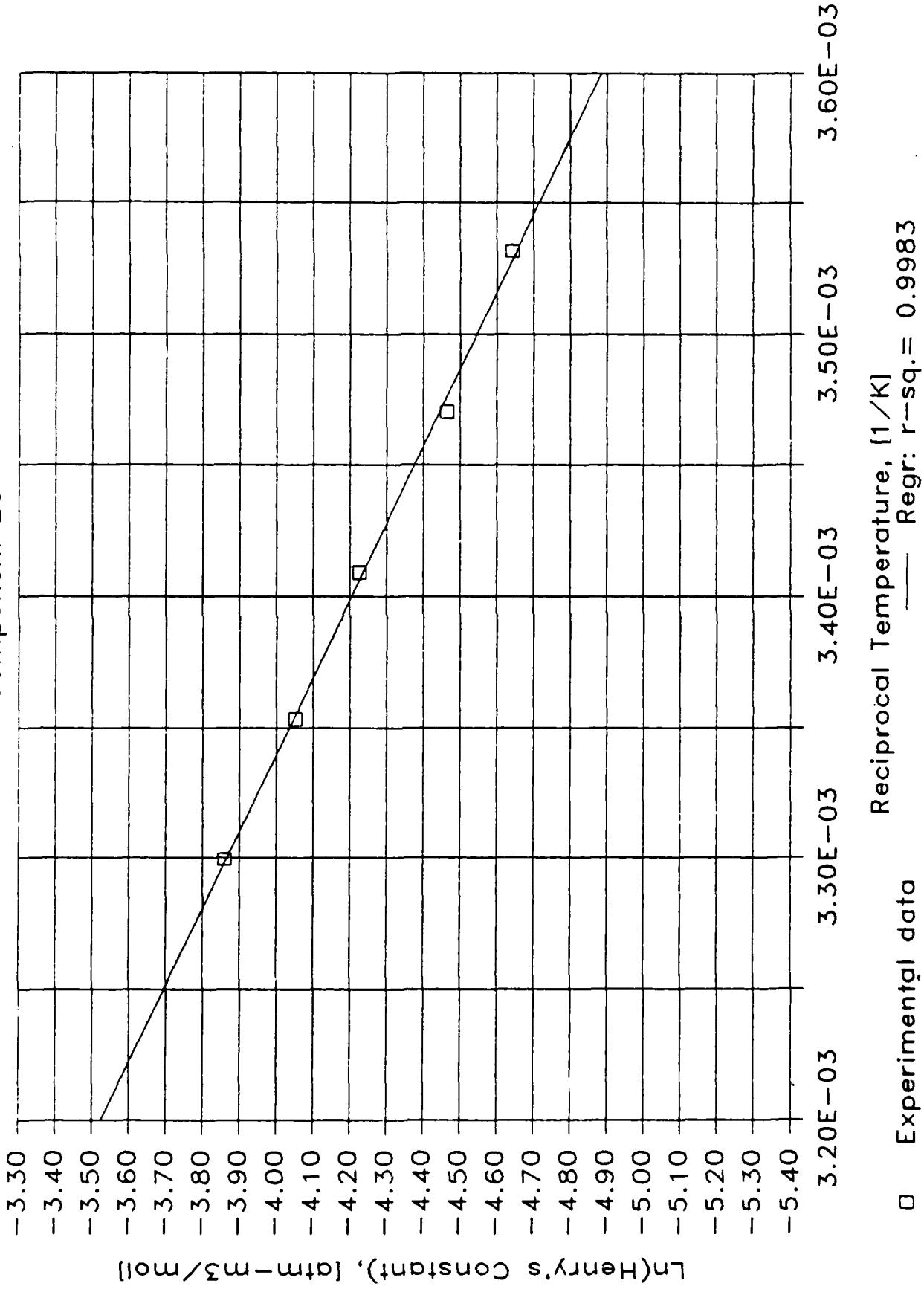
SLOPE = -3.4E+03

Y-INTERCEPT = 7.4E+00

R-SQUARED = 0.9983

TEMPERATURE REGRESSION PLOT

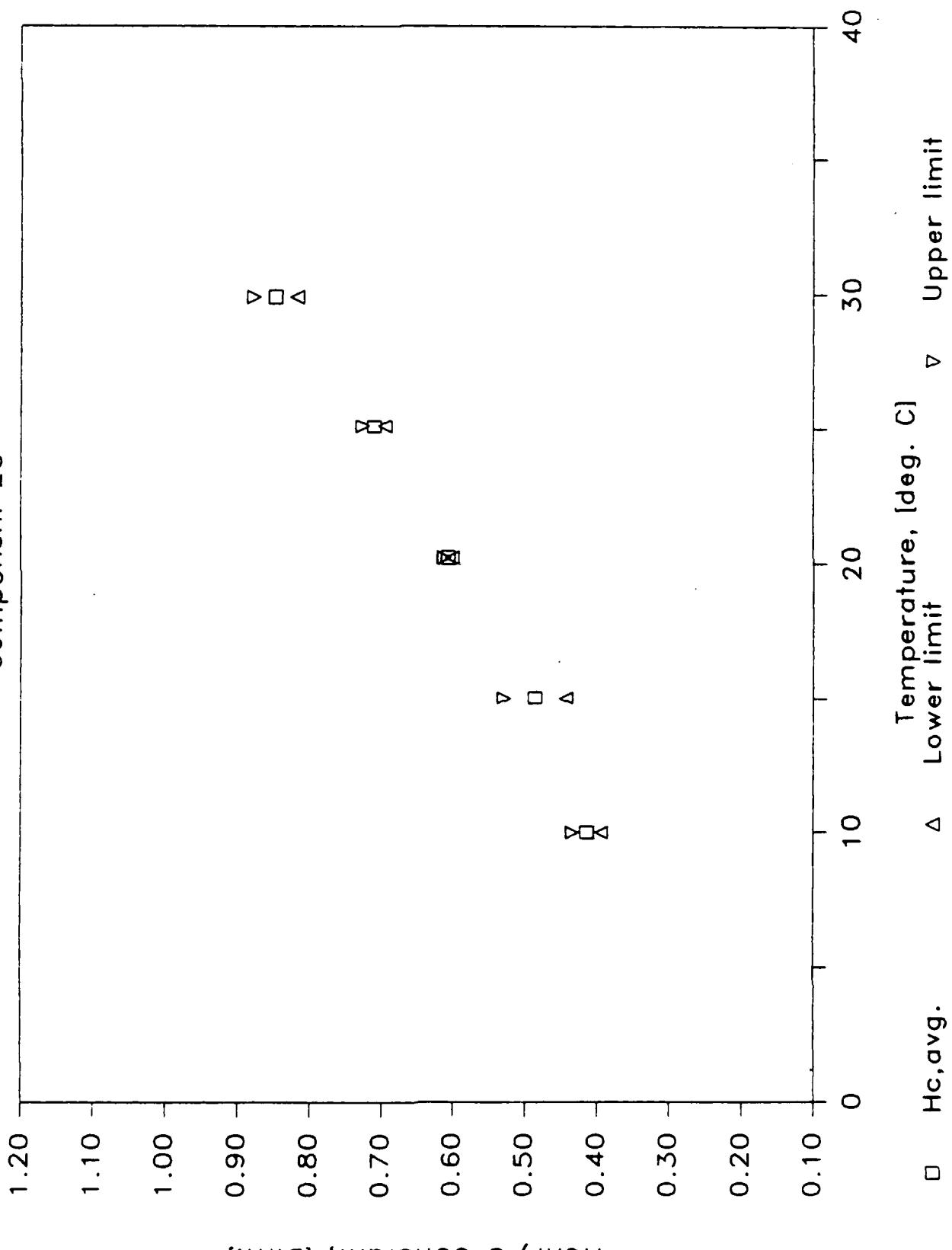
Component 20



Experimentl data

95% CONFIDENCE TEST

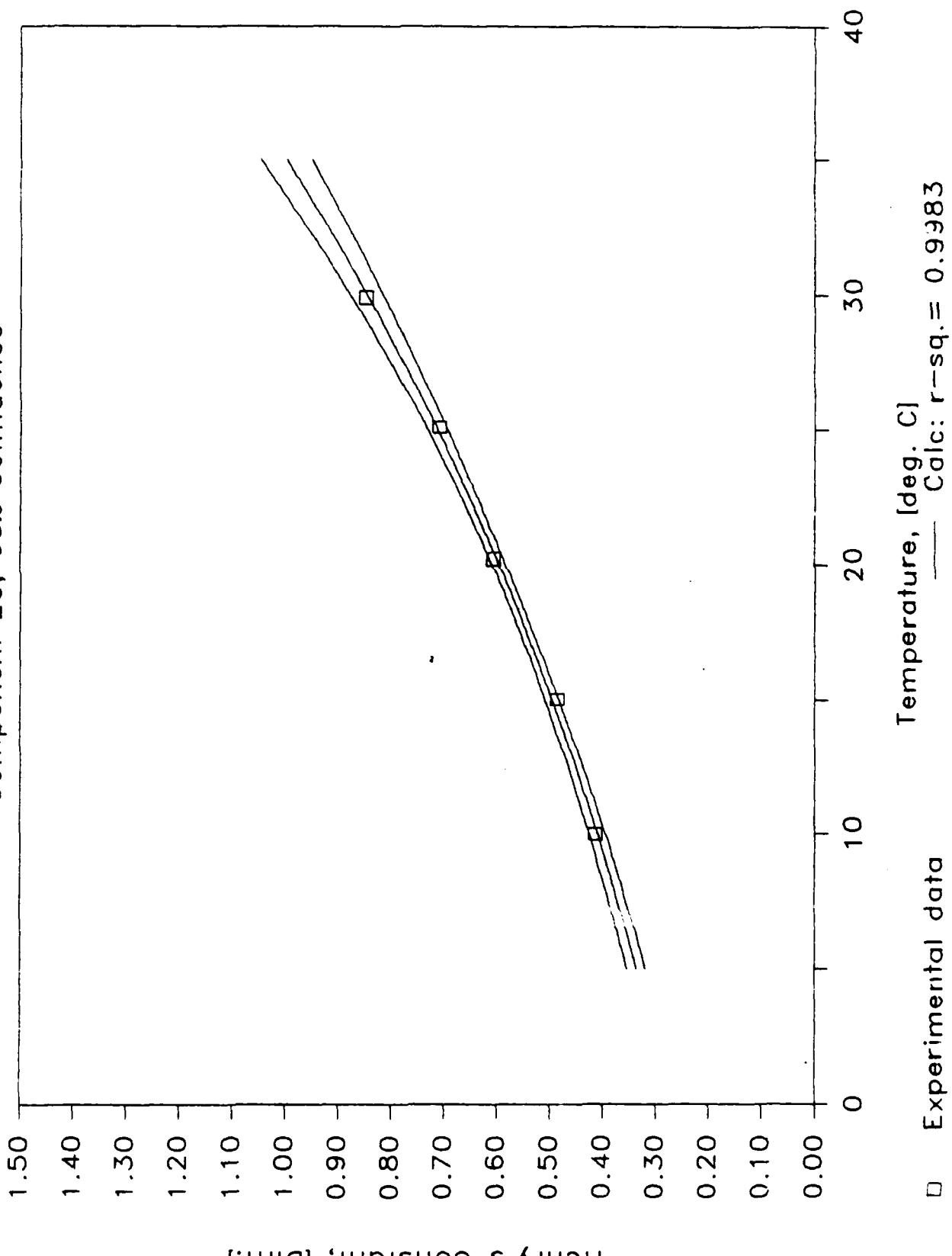
Component 20



183

REGRESSION CONFIDENCE TEST

Component 20, 95% Confidence



□ Experimental data

— Regression line
— 95% Confidence Interval

184

184

86-Nov-86

Results Summary for Component 21

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		13		13		14	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		5		5		5	
Component ID		21		21		21	
Temperature (C)		10		15		20.2	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H, avg: atm-m3/mol		0.0506	1.0E-25	0.0422	1.0E-25	0.0506	1.0E-25
H, avg: atm-mol/mol		64.5		55.3		67.6	
H, avg: atm-m3/mol		1.16E-03	1	9.97E-04	1	1.22E-03	1
H, avg: kPa-m3/mol		0.1178		0.1010		0.1234	
COV, r [std/mean]		11.24		6.24		5.12	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.0564		0.0439		0.0536	
[atm-m3/mol] (2)		0.0526		0.0449		0.0518	
(3)		0.0473		0.0394		0.0494	
(4)		0.0437		0.0404		0.0477	
Injection: (1)		179240		222690		291140	
[Peak Area] (2)		169820		216540		284970	
(3)		986870		1321800		1629700	
(4)		1008900		1313400		1647100	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		14		15	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		5		5	
Component ID		21		21	
Temperature (C)		25		39	
Low Vol (ml)		25		25	
High Vol (ml)		285		285	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.8429	1.0E-25	0.8584	1.0E-25
H, avg: atm-mol/mol		58.2		69.6	
H, avg: atm-m3/mol		1.05E-03	1	1.25E-03	1
H, avg: kPa-m3/mol		0.1063		0.1270	
COV, r [std/mean]		10.91		9.18	
COV, both replic.		—	—	—	—
Observation: (1)		0.8464		0.8584	
[atm-m3/m3] (2)		0.8474		0.8561	
(3)		0.8384		0.8448	
(4)		0.8394		0.8583	
Injection: (1)		344840		410050	
[Peak Area] (2)		327870		397070	
(3)		2815300		2343600	
(4)		2802200		2266300	

Temperature Regression Parameters:

OF POINTS = 5

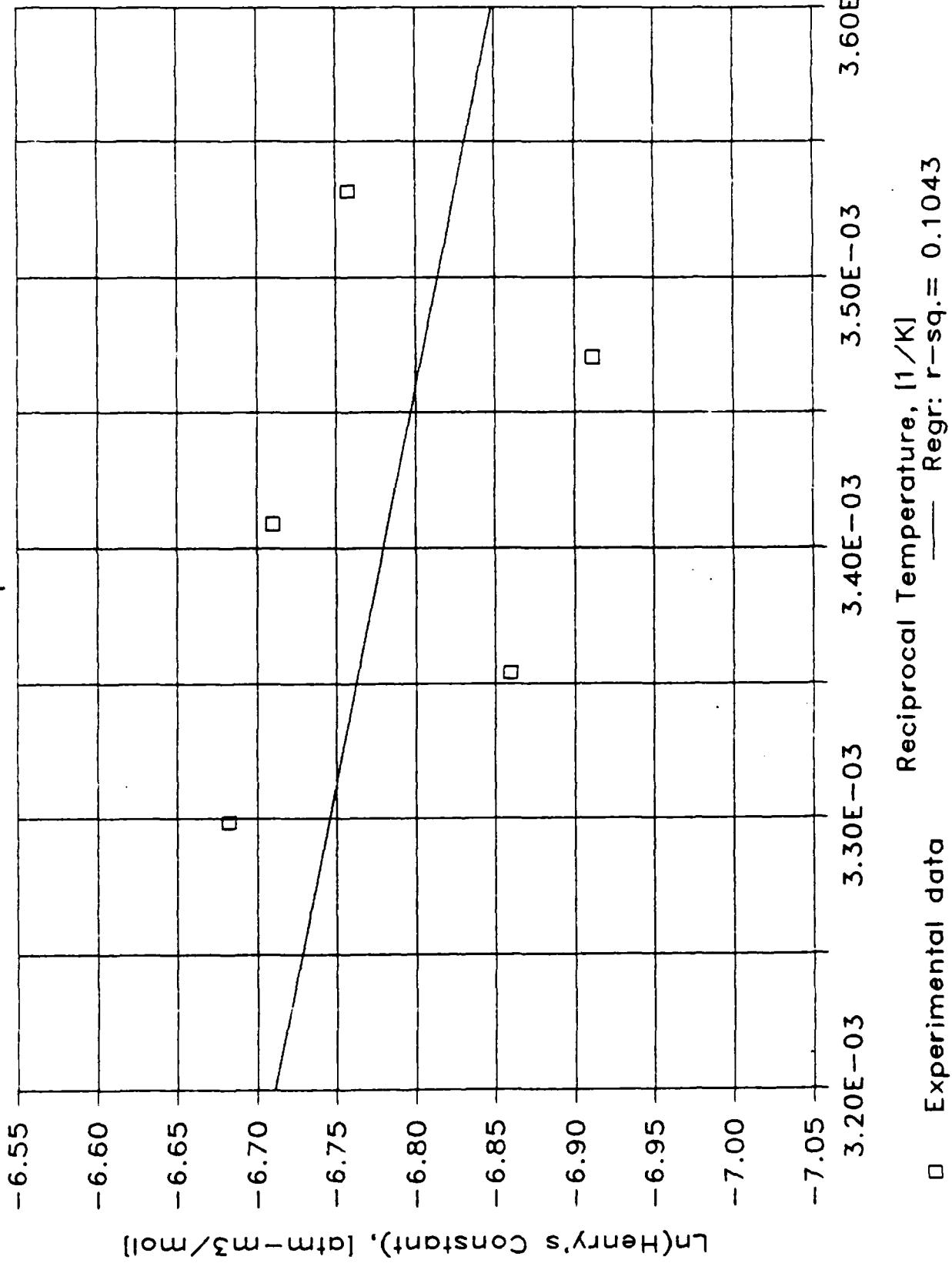
SLOPE = -3.4E+02

Y-INTERCEPT = -5.6E+00

R-SQUARED = 0.1043

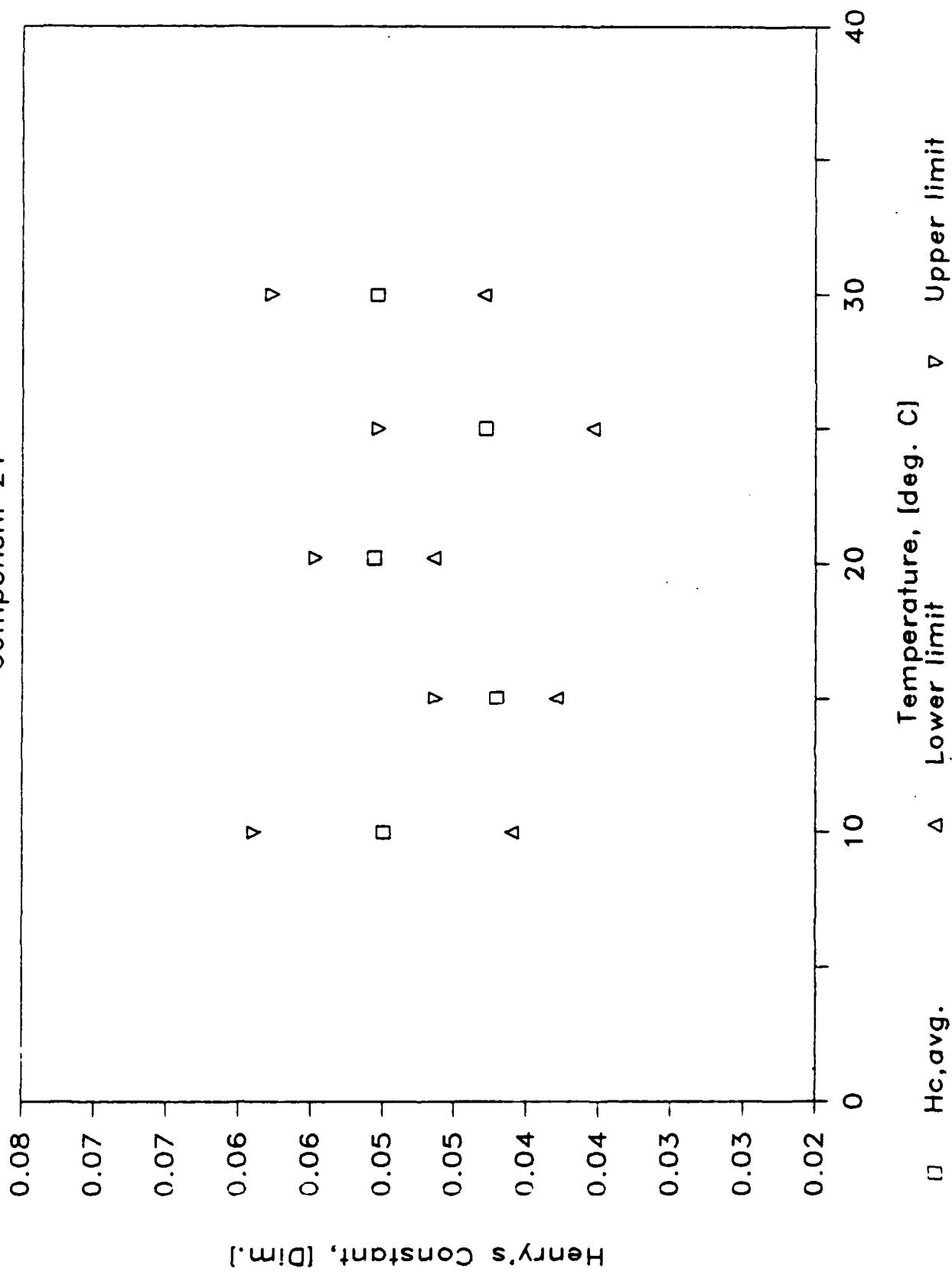
TEMPERATURE REGRESSION PLOT

Component 21



95% CONFIDENCE TEST
Component 21

188

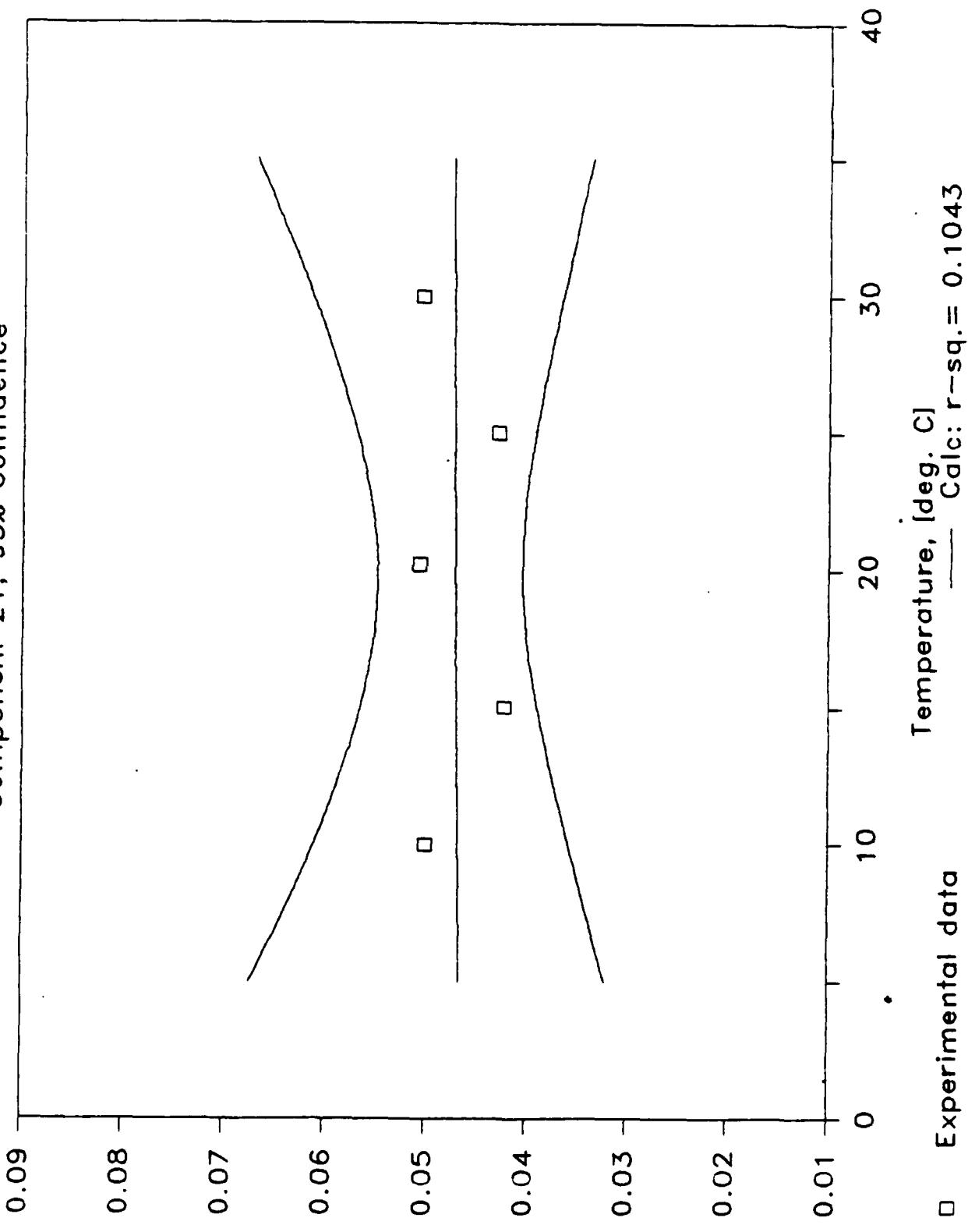


REGRESSION CONFIDENCE TEST

Component 21, 95% Confidence

681

Henry's Constant, [Dim.]



11-Nov-86

Results Summary for Component 121

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	2	2	2	2	3	3
REPLICATE →	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	1		1		1	
Component ID	121		121		121	
Temperature (C)	10.1		15		20	
Low Vol (ml)	25		25		25	
High Vol (ml)	205		205		205	
System Vol (ml)	250		250		250	
H ₄ avg: atm-m ³ /m ³	0.0169	1.0E-25	0.0267	1.0E-25	0.0308	1.0E-25
H ₄ avg: atm-mol/mol	21.8		35.0		41.1	
H ₄ avg: atm-m ³ /mol	3.92E-04	1	6.30E-04	1	7.41E-04	1
H ₄ avg: kPa-m ³ /mol	0.0397		0.0639		0.0751	
COV, r [std/mean]	25.79		7.41		8.64	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0219		0.0282		0.0340	
[atm-m ³ /m ³] (2)	0.0150		0.0285		0.0315	
(3)	0.0187		0.0248		0.0301	
(4)	0.0119		0.0251		0.0276	
Injection: (1)	178840		232120		287330	
[Peak Area] (2)	174610		226620		279850	
(3)	1230800		1527500		1817400	
(4)	1296500		1524200		1848900	

11-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		3		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		1		1	
Component ID		121		121	
Temperature (C)		25		30	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.0371	1.0E-25	0.0535	1.0E-25
H, avg: atm-mol/mol		50.4		73.8	
H, avg: atm-m3/mol		9.08E-04	1	1.33E-03	1
H, avg: kPa-m3/mol		0.0920		0.1348	
COV, r [std/mean]		8.82		2.55	
COV, both replic.		_____		_____	
Observation: (1)		0.0404		0.0552	
[atm-m3/mol]	(2)	0.0395		0.0535	
	(3)	0.0347		0.0535	
	(4)	0.0339		0.0518	
		1			
Injection: (1)		392020		520400	
[Peak Area]	(2)	377940		515300	
	(3)	2378900		2886300	
	(4)	2392500		2914500	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

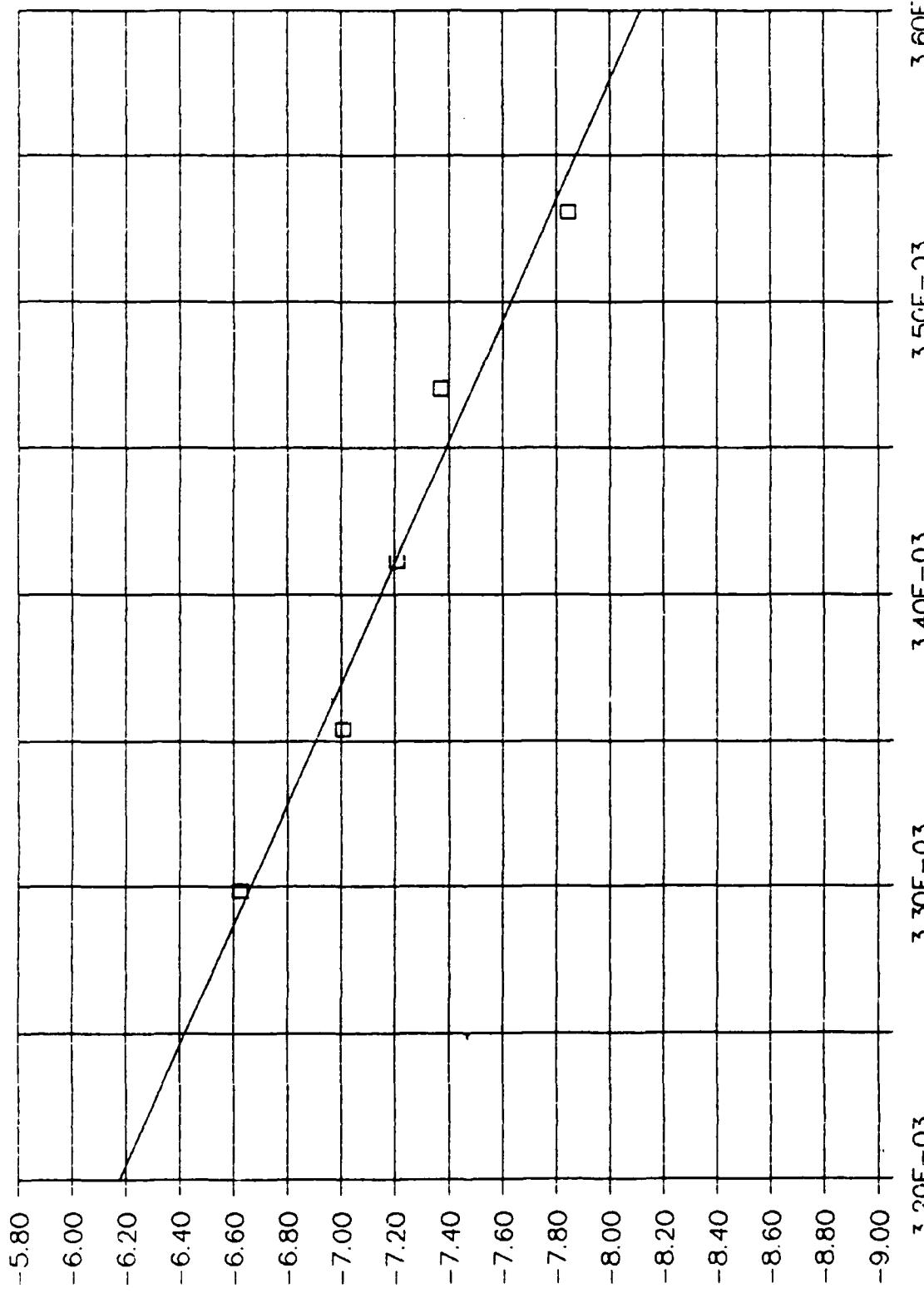
SLOPE = -4.8E+03

Y-INTERCEPT = 9.3E+00

R-SQUARED = 0.9683

TEMPERATURE REGRESSION PLOT

Component 121



□ Experimental data

Reciprocal Temperature, $[1/K]$

Regr: r-sq. = 0.9683

3.60E-03

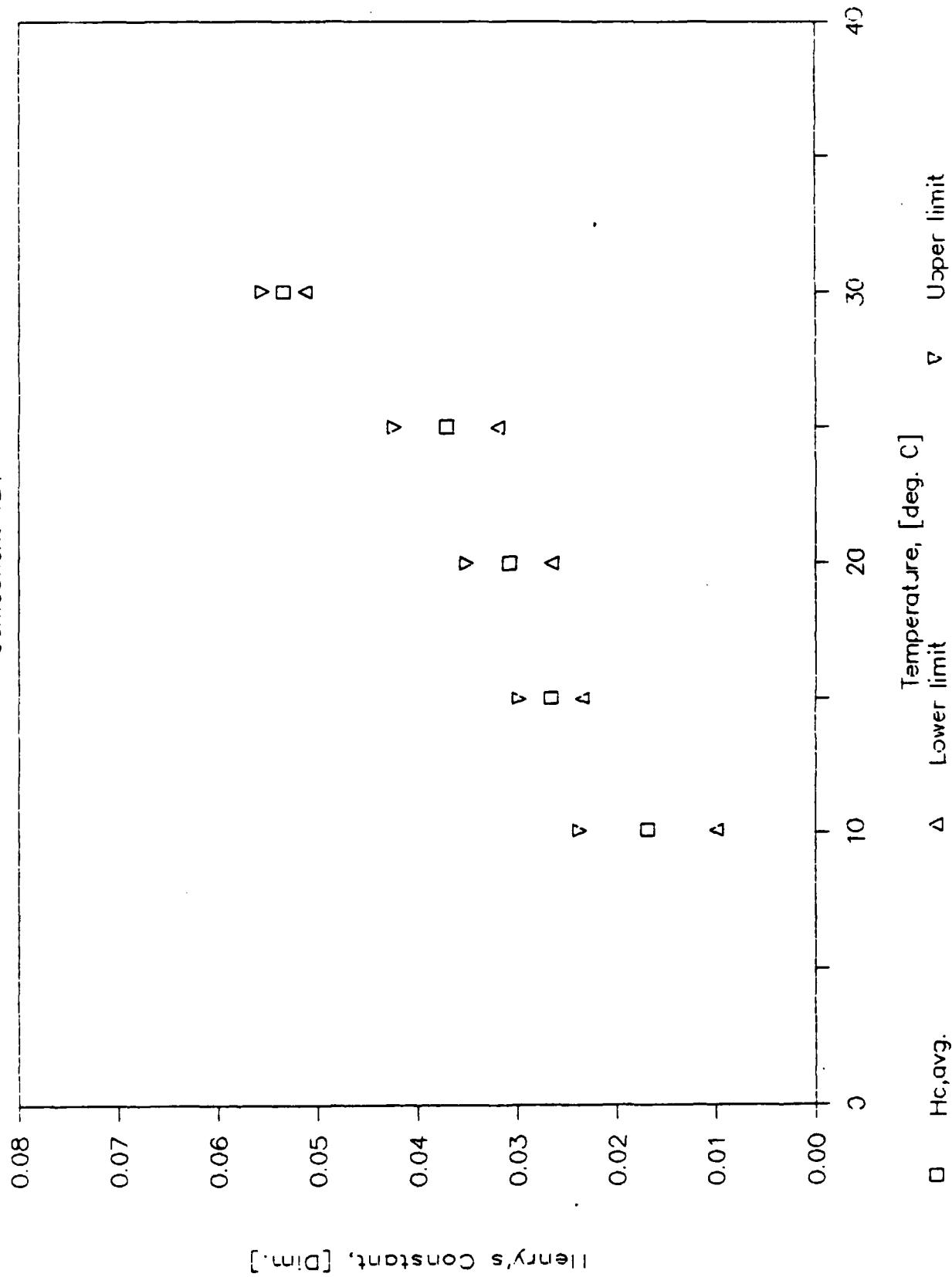
3.50E-03

3.40E-03

3.30E-03

3.20E-03

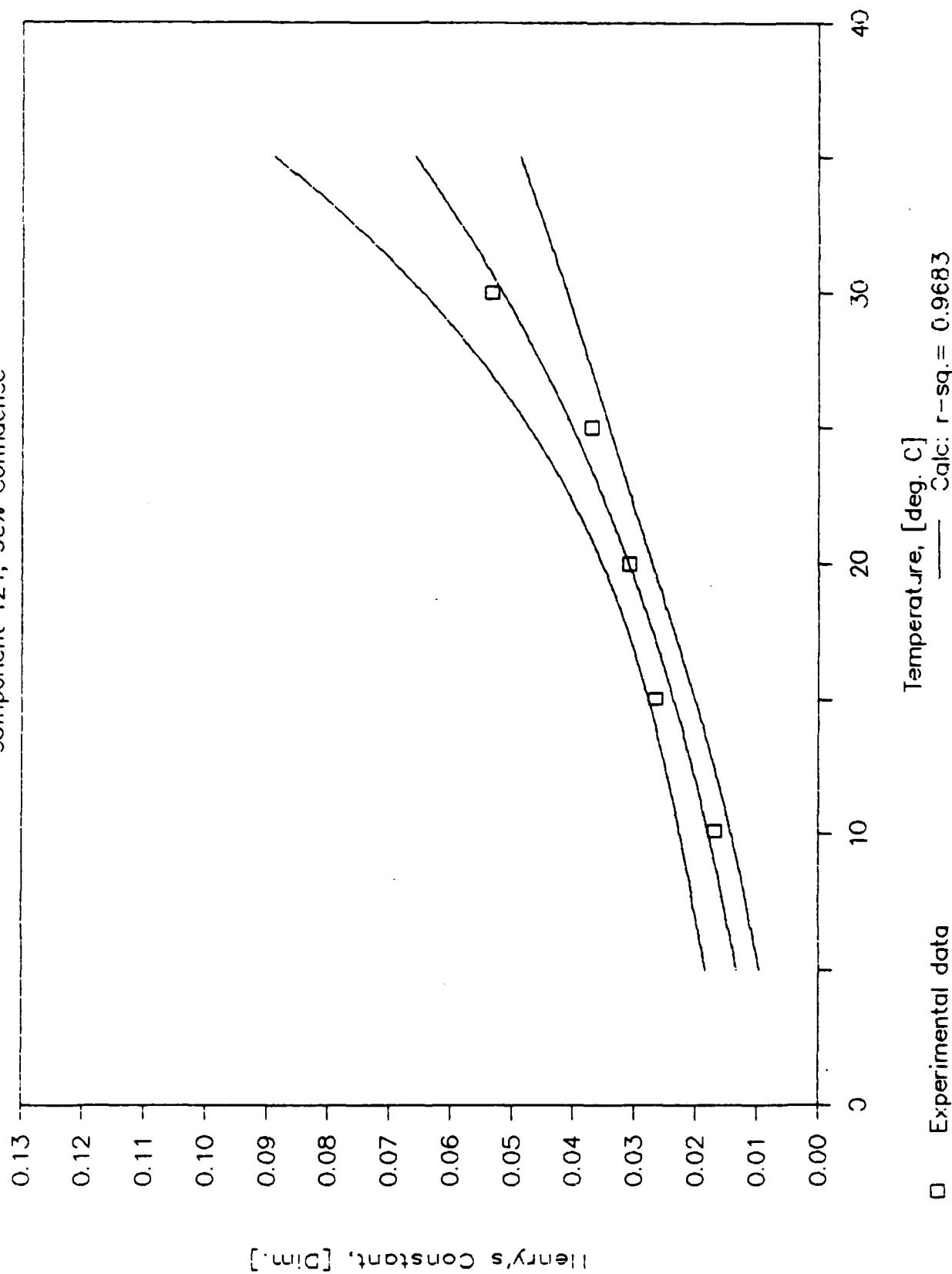
95% CONFIDENCE TEST
Component 121



REGRESSION CONFIDENCE TEST

Component 121, 95% Confidence

194



06-Nov-86

Results Summary for Component 22

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		2		2		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		6		6		6	
Component ID		22		22		22	
Temperature (C)		9.9		15		28.1	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H ₄ avg: atm-m3/m3		0.1164	1.0E-25	0.1379	1.0E-25	0.1494	1.0E-25
H ₄ avg: atm-mol/mol		150.1		181.0		199.6	
H ₄ avg: atm-m3/mol		2.70E-03	1	3.26E-03	1	3.60E-03	1
H ₄ avg: kPa-m3/mol		0.2740		0.3304		0.3643	
COV, r [std/mean]		3.86		4.26		0.17	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.1139		0.1452		0.1497	
[atm-m3/m3] (2)		0.1214		0.1379		0.1493	
(3)		0.1115		0.1378		0.1495	
(4)		0.1189		0.1308		0.1491	
Injection: (1)		976550		1158000		1321600	
[Peak Area] (2)		966690		1127300		1320600	
(3)		4052500		4251200		4768600	
(4)		3929000		4368500		4775300	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		3		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		6		6	
Component ID		22		22	
Temperature (C)		25		29.9	
Low Vol (ml)		25		25	
High Vol (ml)		285		285	
System Vol (ml)		250		250	
H _{avg} : atm-m ³ /mol		0.1858	1.0E-25	0.2311	1.0E-25
H _{avg} : atm-mol/mol		252.3		319.0	
H _{avg} : atm-m ³ /mol		4.54E-03	1	5.75E-03	1
H _{avg} : kPa-m ³ /mol		0.4685		0.5823	
COV, r [std/mean]		4.00		6.32	
COV, both replic.		—		—	
Observation: (1)		0.1923		0.2460	
[atm-m ³ /mol]	(2)	0.1794		0.2410	
	(3)	0.1921		0.2210	
	(4)	0.1792		0.2164	
Injection:	(1)	1689800		2262600	
[Peak Area]	(2)	1688500		2115000	
	(3)	5288300		6884400	
	(4)	5507600		6164000	

Temperature Regression Parameters:

OF POINTS = 5

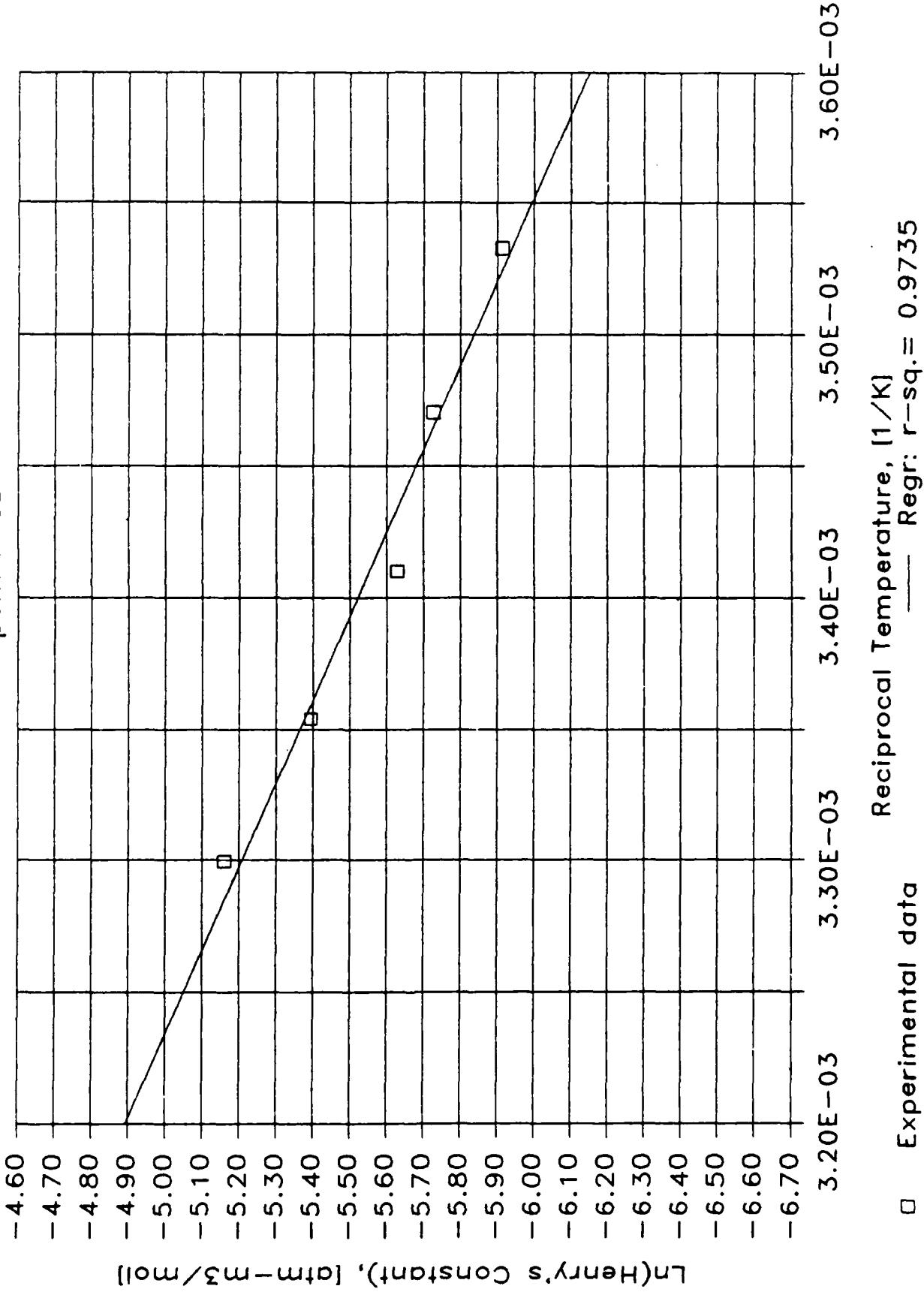
SLOPE = -3.1E+03

Y-INTERCEPT = 5.2E+00

R-SQUARED = 0.9735

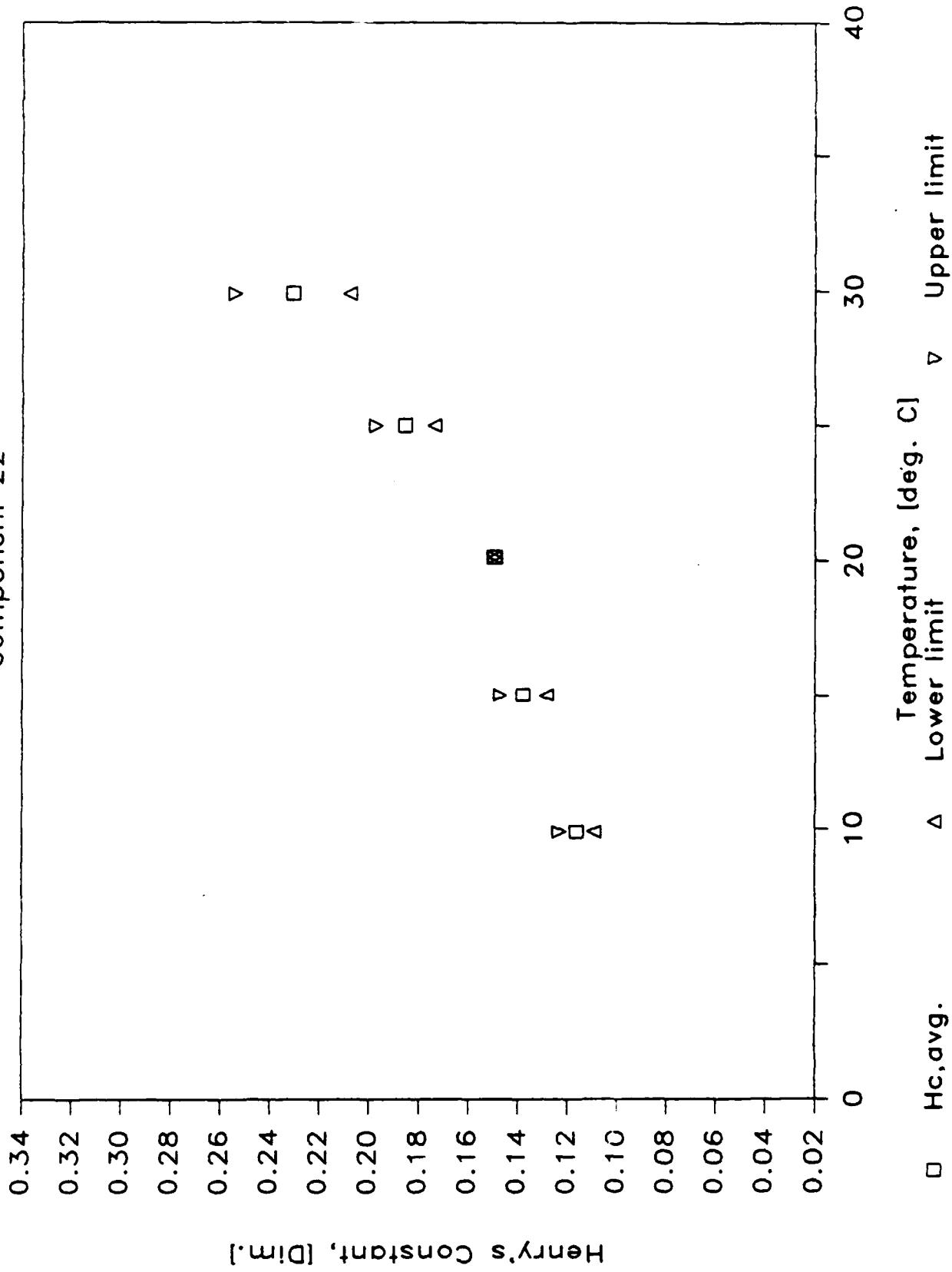
TEMPERATURE REGRESSION PLOT

Component 22

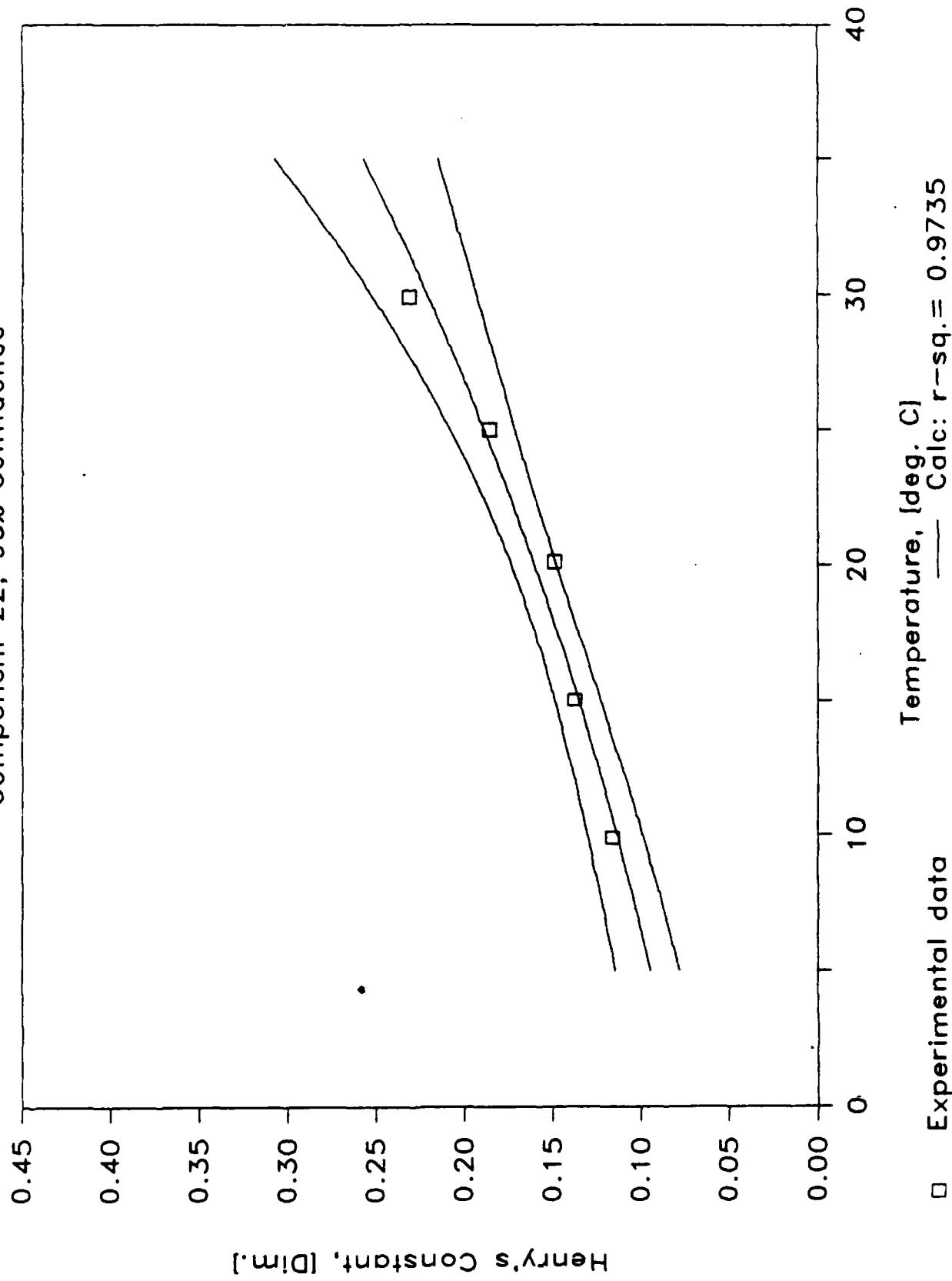


95% CONFIDENCE TEST
Component 22

198



REGRESSION CONFIDENCE TEST
Component 22, 95% Confidence



06-Nov-86

Results Summary for Component 23

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	6	No. 1 No. 2	6	No. 1 No. 2	7	No. 1 No. 2
REPLICATE →						
Group No.		6		6		6
Component ID		23		23		23
Temperature (C)		9.9		15		20.1
Low Vol (ml)		25		25		25
High Vol (ml)		205		205		205
System Vol (ml)		250		250		250
H, avg: atm-m3/mol	0.2547	1.0E-25	0.2980	1.0E-25	0.3559	1.0E-25
H, avg: atm-mol/mol	328.4		391.1		475.4	
H, avg: atm-m3/mol	5.92E-03	1	7.05E-03	1	8.57E-03	1
H, avg: kPa-m3/mol	0.5995		0.7140		0.8679	
COV, r [std/mean]	5.24		0.79		4.48	
COV, both replic.	—	—	—	—	—	—
Observation: (1)	0.2695		0.2991		0.3755	
[atm-m3/mol] (2)	0.2619		0.3007		0.3585	
(3)	0.2473		0.2953		0.3529	
(4)	0.2482		0.2970		0.3368	
Injection: (1)	2123400		2451600		2964300	
[Peak Area] (2)	2009000		2431100		2839900	
(3)	5383700		5883300		6000200	
(4)	5484600		5781800		6293300	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		7		7	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		6		6	
Component ID		23		23	
Temperature (C)		25		29.9	
Low Vol (ml)		25		25	
High Vol (ml)		265		265	
System Vol (ml)		250		250	
H ₄ avg: atm-m ³ /mol		0.3862	1.0E-25	0.4879	1.0E-25
H ₄ avg: atm-mol/mol		524.5		673.4	
H ₄ avg: atm-m ³ /mol		9.45E-03	1	1.21E-02	1
H ₄ avg: kPa-m ³ /mol		0.9575		1.2293	
COV, r [std/mean]		1.30		2.82	
COV, both replic.		—	—	—	—
Observation: (1)		0.3921		0.4712	
[atm-m ³ /mol]	(2)	0.3881		0.4861	
	(3)	0.3843		0.4894	
	(4)	0.3804		0.5048	
Injection: (1)		3506400		4208800	
[Peak Area]	(2)	3457500		4324500	
	(3)	6895400		7256300	
	(4)	6944200		7106100	

Temperature Regression Parameters:

OF POINTS = 5

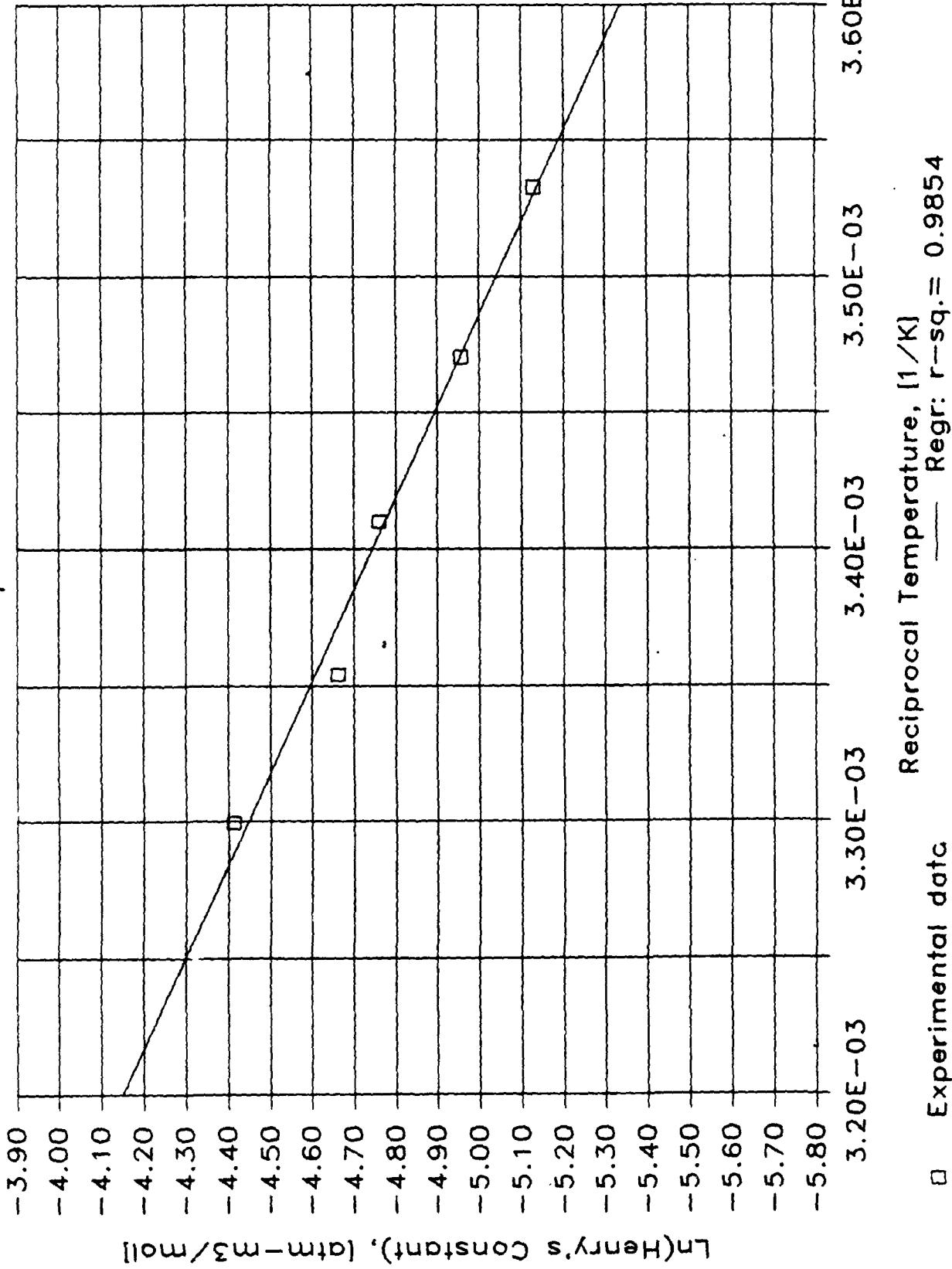
SLOPE = -3.0E+03

Y-INTERCEPT = 5.3E+00

R-SQUARED = 0.9854

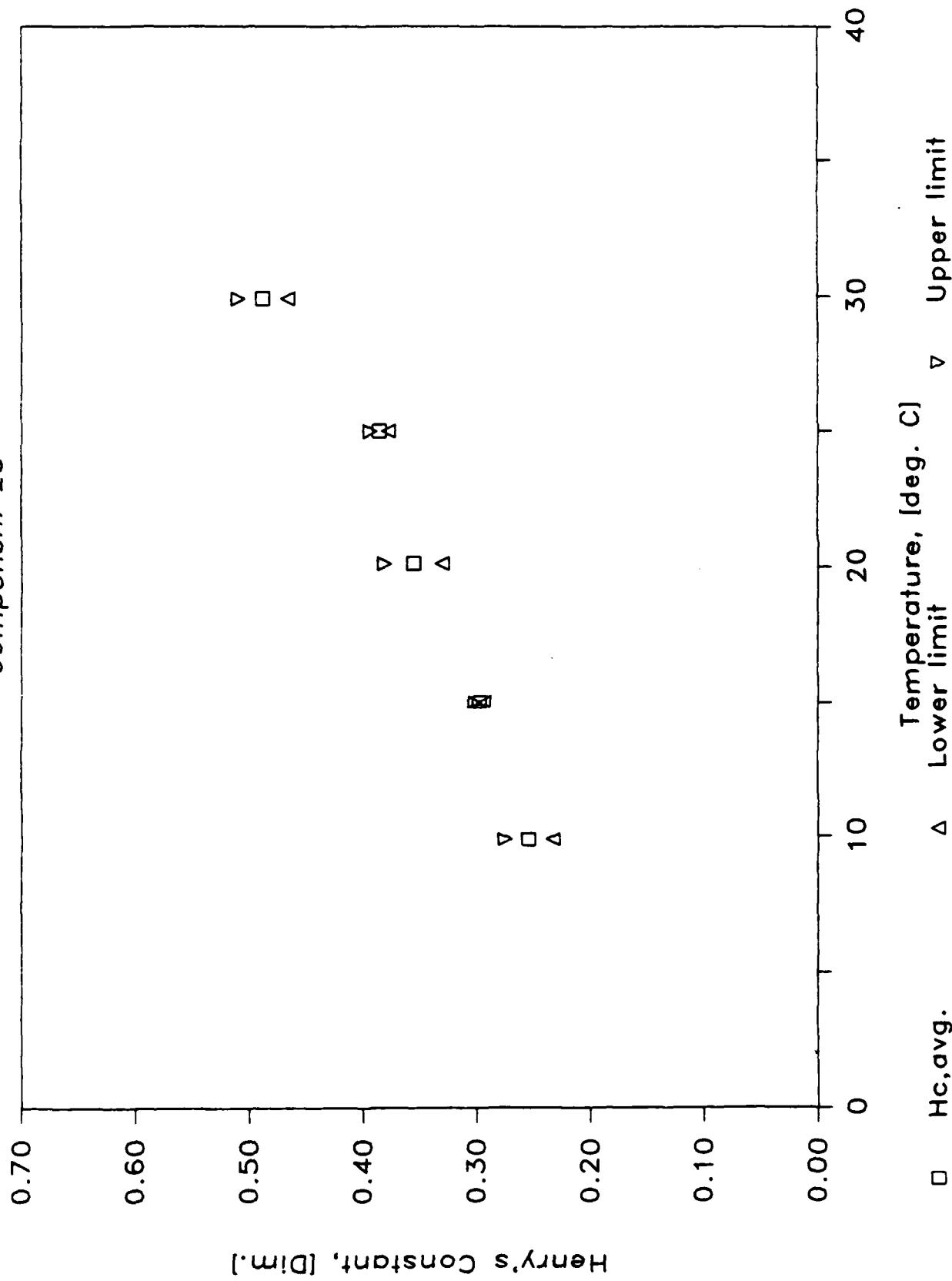
TEMPERATURE REGRESSION PLOT

Component 23

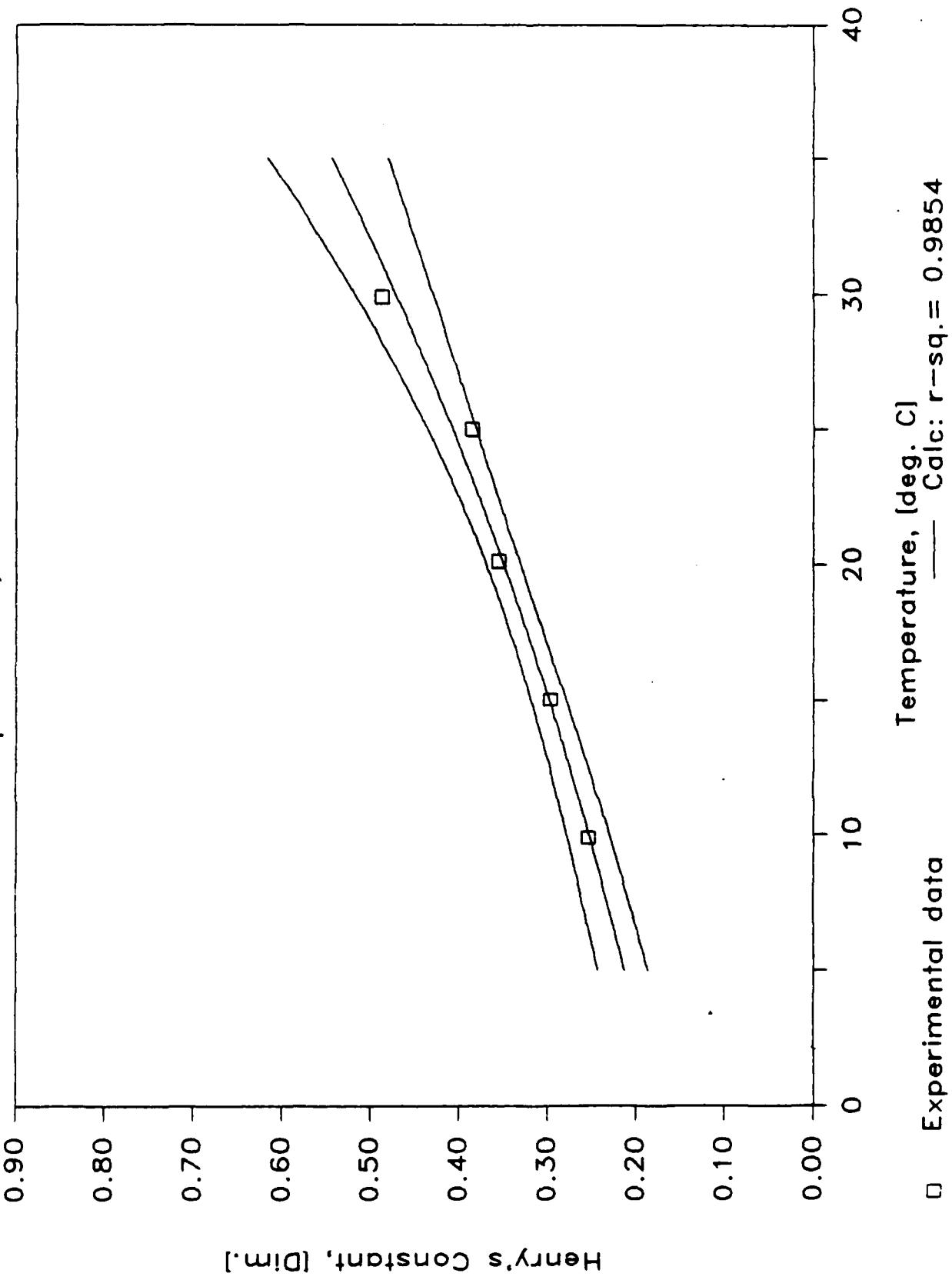


95% CONFIDENCE TEST Component 2³

203



REGRESSION CONFIDENCE TEST
Component 23, 95% Confidence



06-Nov-86

Results Summary for Component 24

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		10		10		11	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		6		6		6	
Component ID		24		24		24	
Temperature (C)		9.9		15		20.1	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H, avg: atm-m3/m3		0.3644	1.0E-25	0.4702	1.0E-25	0.5840	1.0E-25
H, avg: atm-mol/mol		469.8		617.1		788.0	
H, avg: atm-m3/mol		8.46E-03	1	1.11E-02	1	1.41E-02	1
H, avg: kPa-m3/mol		0.8576		1.1266		1.4239	
COV, r [std/mean]		4.19		4.99		1.52	
COV, both replic.							
Observation: (1)		0.3713		0.4922		0.5829	
[atm-m3/m3] (2)		0.3819		0.4887		0.5949	
(3)		0.3472		0.4516		0.5732	
(4)		0.3573		0.4483		0.5849	
Injection: (1)		582400		973110		1192400	
[Peak Area] (2)		556140		914900		1177900	
(3)		1189800		1628300		1765700	
(4)		1166700		1636700		1739800	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		11		11	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		6		6	
Component ID		24		24	
Temperature (C)		25		29.9	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H ₄ avg: atm-m ³ /m ³		0.6970	1.0E-25	0.9839	1.0E-25
H ₄ avg: atm-mol/mol		946.5		1358.1	
H ₄ avg: atm-m ³ /mol		1.71E-02	1	2.45E-02	1
H ₄ avg: kPa-m ³ /mol		1.7278		2.4793	
COV, r [std/mean]		1.65		4.04	
COV, both replic.		_____		_____	
Observation: (1)		0.6973		1.0259	
[atm-m ³ /m ³] (2)		0.7112		0.9584	
(3)		0.6829		1.0088	
(4)		0.6365		0.9425	
Injection: (1)		1107000		1129300	
[Peak Area] (2)		1090300		1115700	
(3)		1438600		1108700	
(4)		1418100		1164400	

Temperature Regression Parameters:

OF POINTS = 5

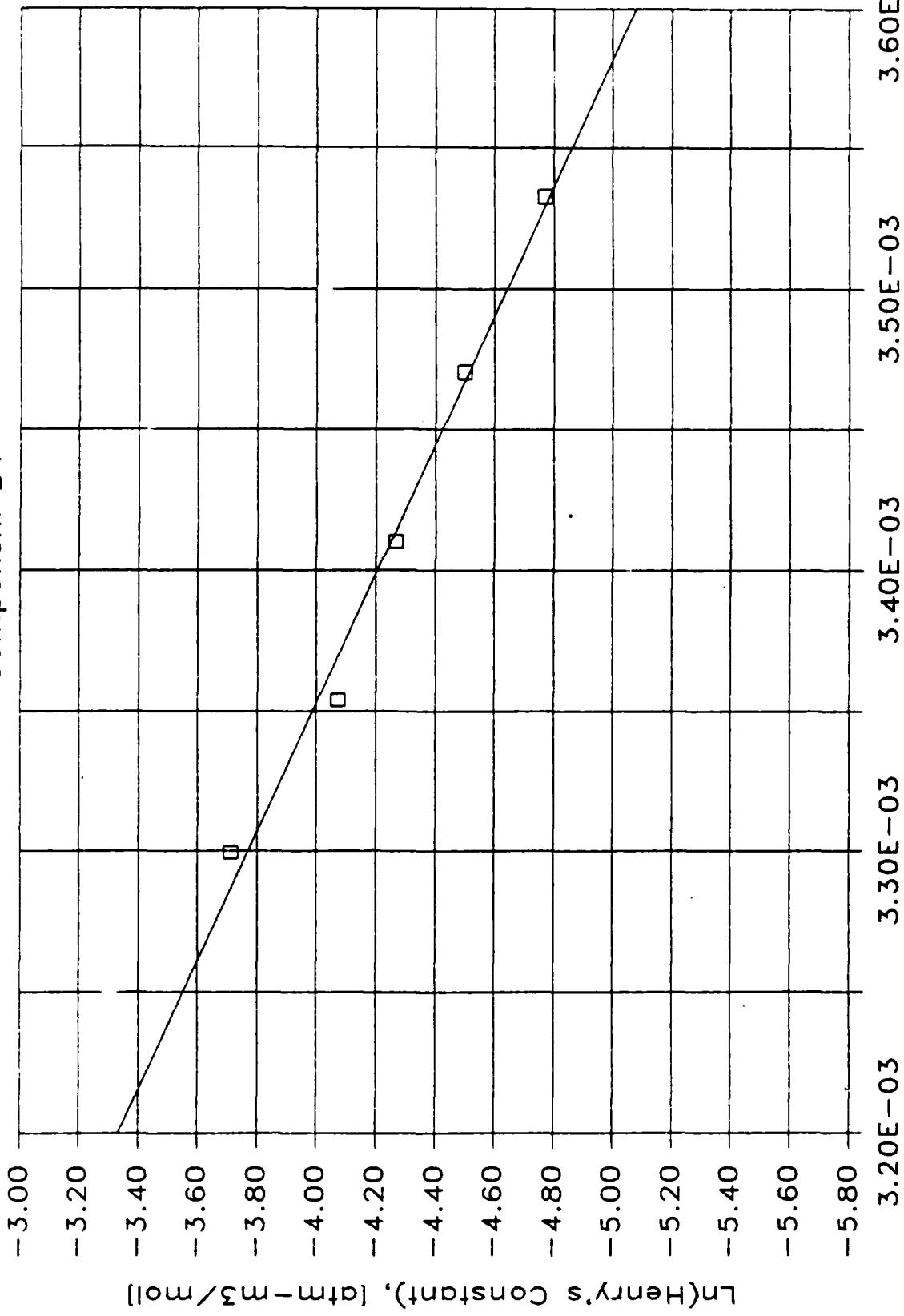
SLOPE = -4.4E+03

Y-INTERCEPT = 1.1E+01

R-SQUARED = 0.9872

TEMPERATURE REGRESSION PLOT

Component 24

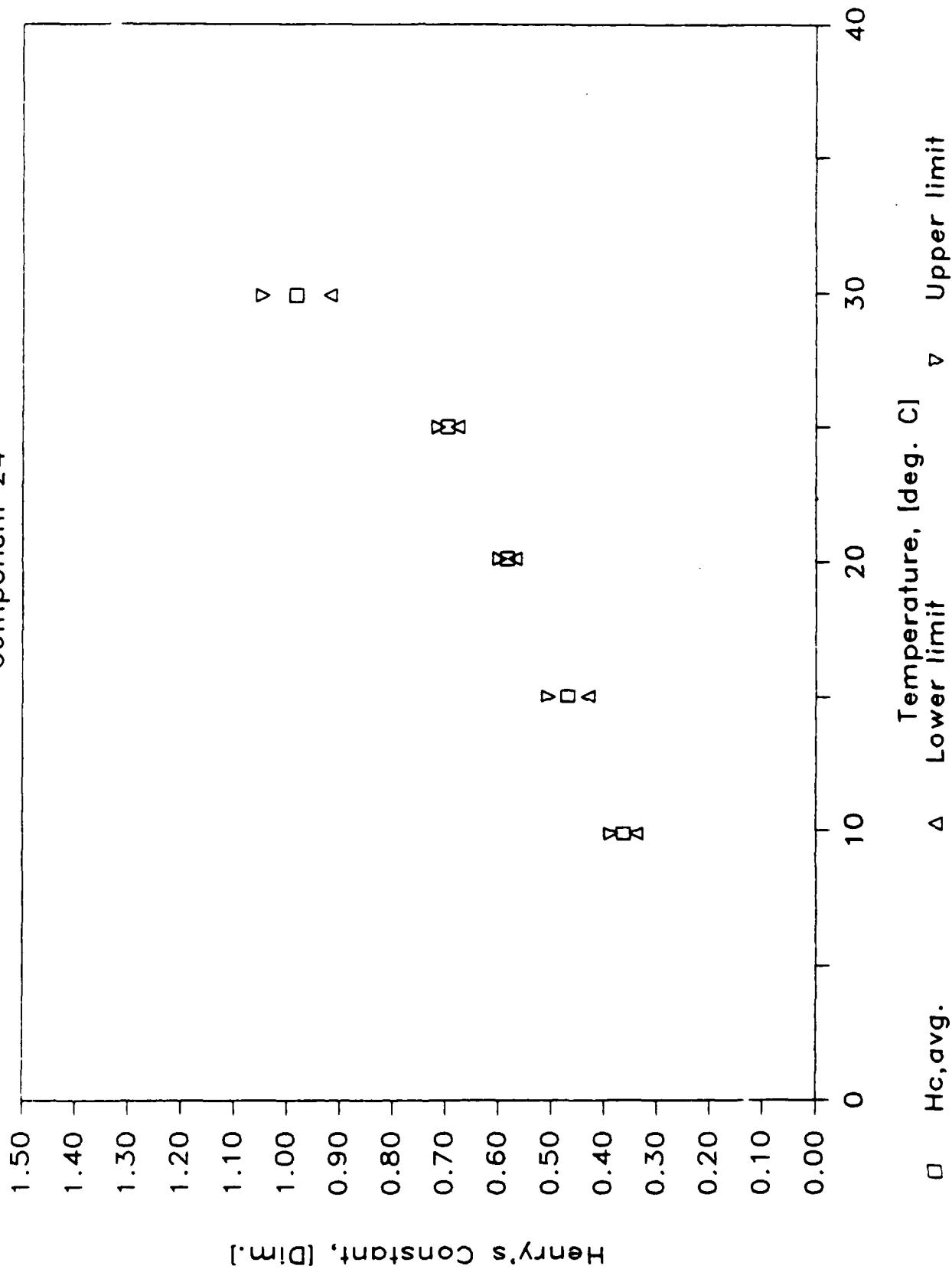


□ Experimental data

— Reciprocal Temperature, [1/K]
Regr: r-sq. = 0.9872

95% CONFIDENCE TEST
Component 24

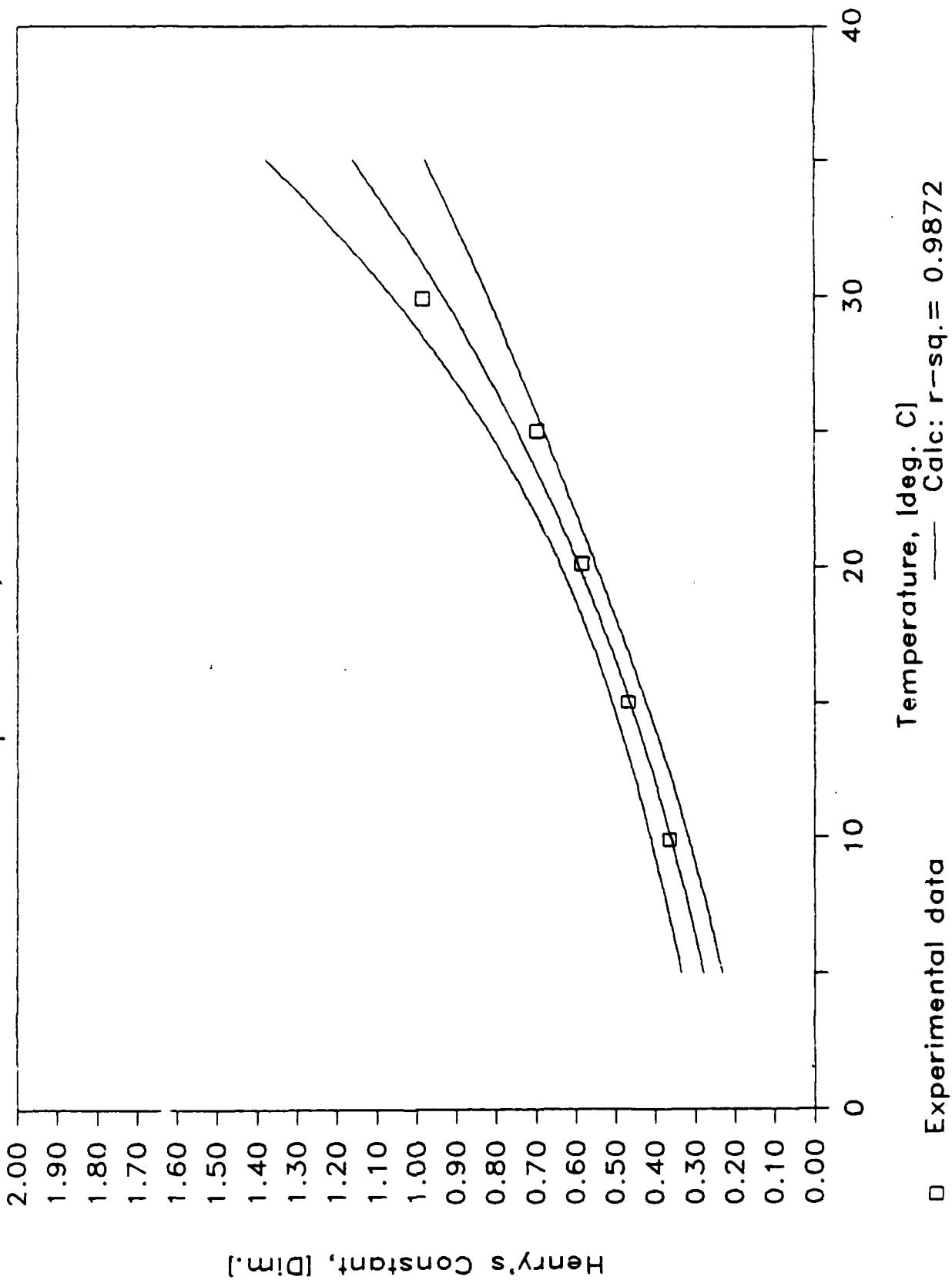
208



REGRESSION CONFIDENCE TEST

Component 24, 95% Confidence

209



06-Nov-86

Results Summary for Component 25

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		14		14		15	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		6		6		6	
Component ID		25		25		25	
Temperature (C)		9.9		15		20.1	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H ₄ avg: atm-m ³ /m ³		0.2317	1.0E-25	0.2823	1.0E-25	0.3498	1.0E-25
H ₄ avg: atm-mol/mol		298.7		370.5		467.2	
H ₄ avg: atm-m ³ /mol		5.38E-03	1	6.68E-03	1	8.42E-03	1
H ₄ avg: kPa-m ³ /mol		0.5452		0.6763		0.8530	
COV, r [std/mean]		3.85		4.41		3.72	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.2290		0.2796		0.3579	
[atm-m ³ /m ³] (2)		0.2424		0.2975		0.3636	
(3)		0.2211		0.2674		0.3362	
(4)		0.2342		0.2847		0.3416	
Injection: (1)		210770		296900		375060	
[Peak Area] (2)		206250		288350		359280	
(3)		593030		734820		785850	
(4)		572190		705270		777310	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		15		15	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		6		6	
Component ID		25		25	
Temperature (C)		25		29.9	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.4149 1.0E-25		0.5164 1.0E-25	
H, avg: atm-mol/mol		563.5		712.8	
H, avg: atm-m3/mol		1.02E-02	1	1.28E-02	1
H, avg: kPa-m3/mol		1.0286		1.3811	
COV, r [std/mean]		1.25		1.84	
COV, both replic.		_____		_____	
Observation: (1)		0.4182		0.5278	
[atm-m3/m3] (2)		0.4203		0.5184	
(3)		0.4095		0.5142	
(4)		0.4116		0.5050	
Injection: (1)		398990		463500	
[Peak Area] (2)		393110		454810	
(3)		749820		737510	
(4)		747130		747140	

Temperature Regression Parameters:

OF POINTS = 5

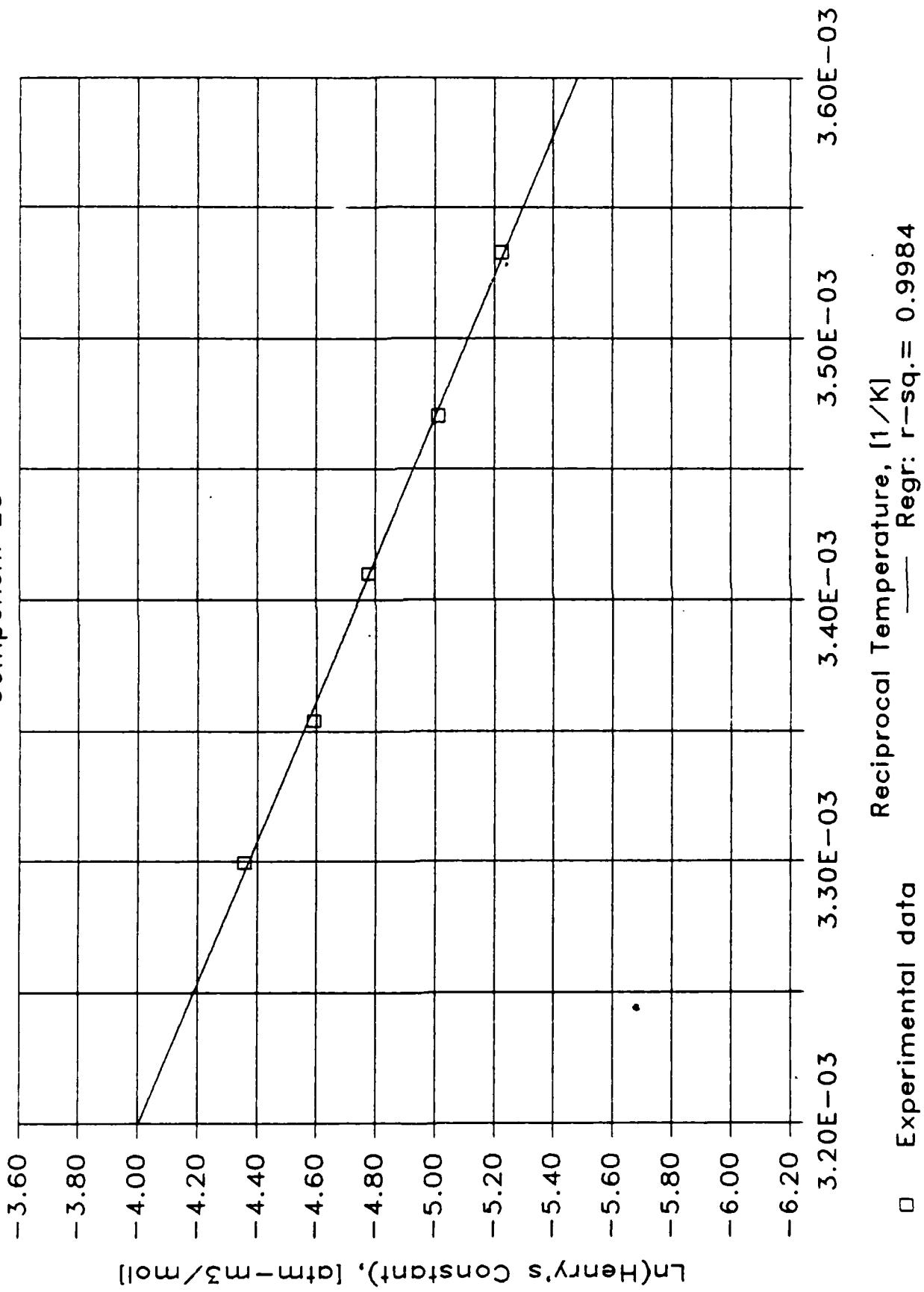
SLOPE = -3.7E+03

Y-INTERCEPT = 7.8E+00

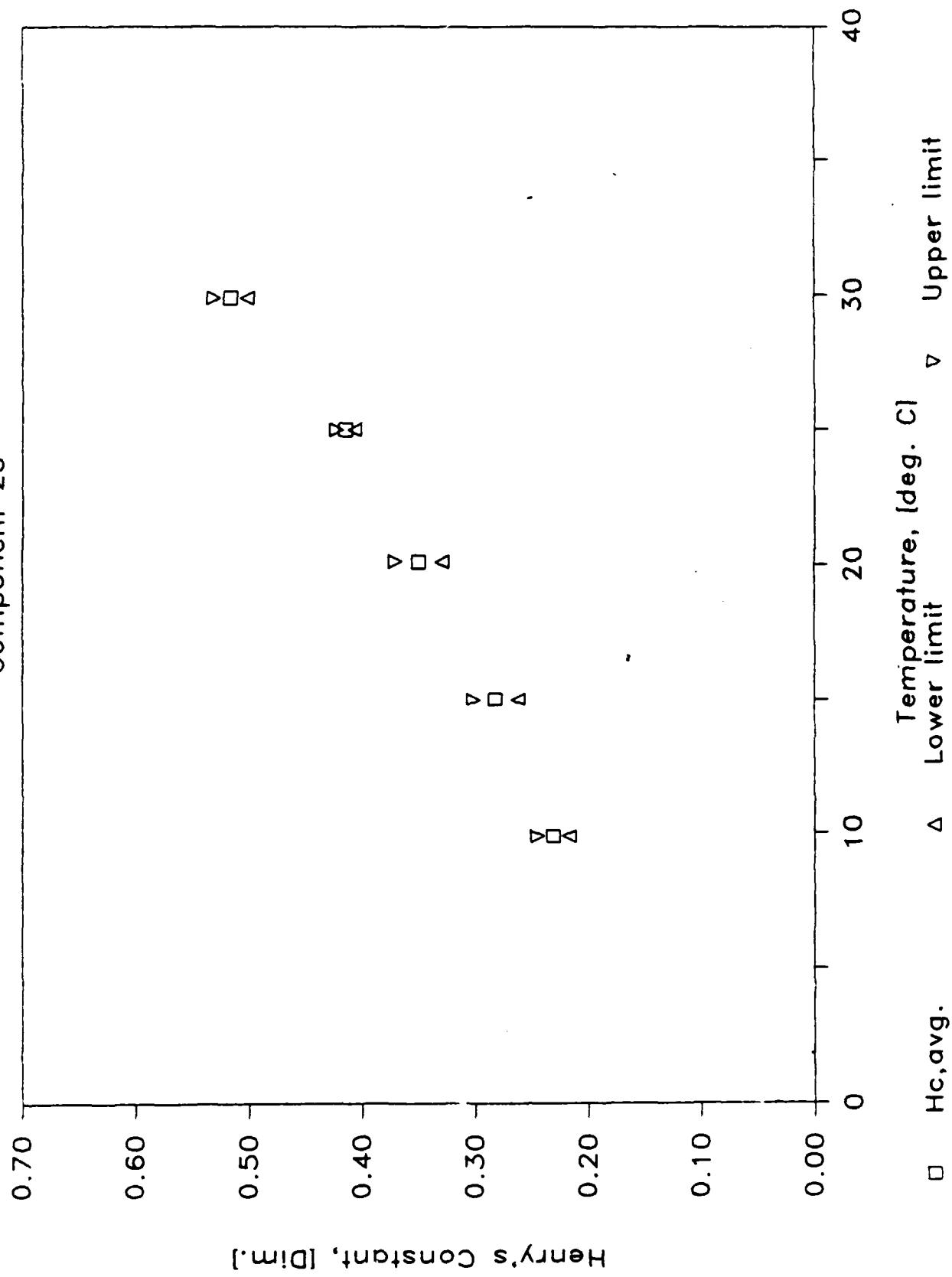
R-SQUARED = 0.9984

TEMPERATURE REGRESSION PLOT

Component 25

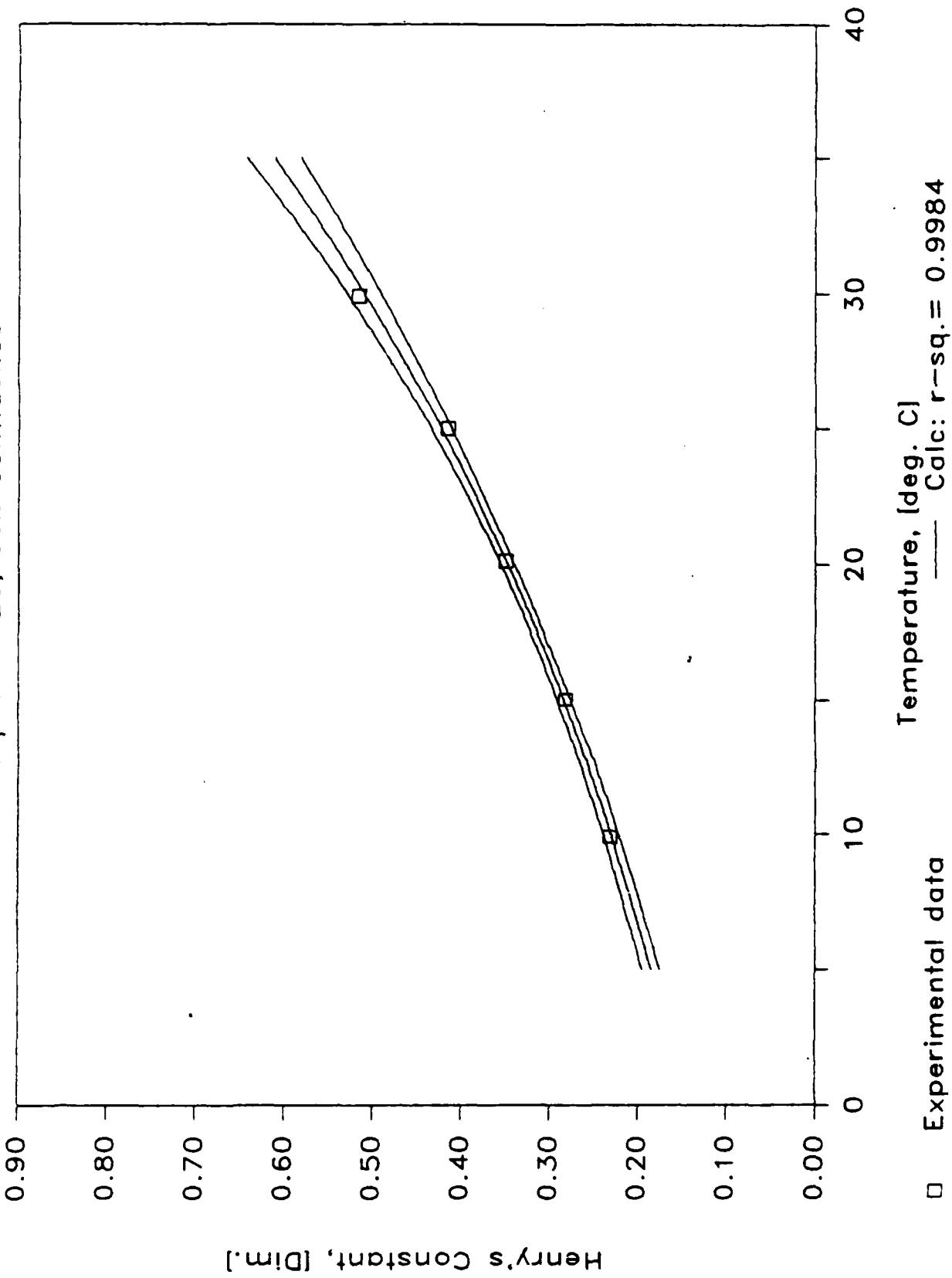


95% CONFIDENCE TEST
Component 25



REGRESSION CONFIDENCE TEST

Component 25, 95% Confidence



86-Nov-86

Results Summary for Component 26

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE →						
Group No.	7		7		7	
Component ID	26		26		26	
Temperature (C)	10		14.9		20.2	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	0.1105	1.0E-25	0.0125	1.0E-25	0.0258	1.0E-25
H, avg: atm-mol/mol	142.5		16.3		34.5	
H, avg: atm-m3/mol	2.57E-03	1	2.94E-04	1	6.21E-04	1
H, avg: kPa-m3/mol	0.2601		0.0298		0.0629	
COV, r [std/mean]	38.57		74.63		12.93	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.1514		0.0095		0.0298	
[atm-m3/mol] (2)	0.1430		0.0237		0.0266	
(3)	0.0769		0.0016		0.0249	
(4)	0.0707		0.0150		0.0218	
Injection: (1)	60315		41886		53285	
[Peak Area] (2)	45313		39600		51772	
(3)	205828		274600		307810	
(4)	211730		250920		313720	

86-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	9	1	1	2
REPLICATE →	No. 1	No. 2	No. 1	No. 2
Group No.	7		7	
Component ID	26		26	
Temperature (C)	25		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H _a avg: atm-m3/mol	0.0494	1.0E-25	0.0327	1.0E-25
H _a avg: atm-mol/mol	67.1		45.2	
H _a avg: atm-m3/mol	1.21E-03	1	8.14E-04	1
H _a avg: kPa-m3/mol	0.1225		0.0825	
COV, r [std/mean]	29.07		6.50	
COV, both replic.	_____		_____	
Observation: (1)	0.0339		0.0352	
[atm-m3/mol] (2)	0.0595		0.0336	
(3)	0.0391		0.0319	
(4)	0.0352		0.0383	
Injection: (1)	91700		98912	
[Peak Area] (2)	80707		97049	
(3)	442400		554030	
(4)	451930		559110	

Temperature Regression Parameters:

OF POINTS = 5

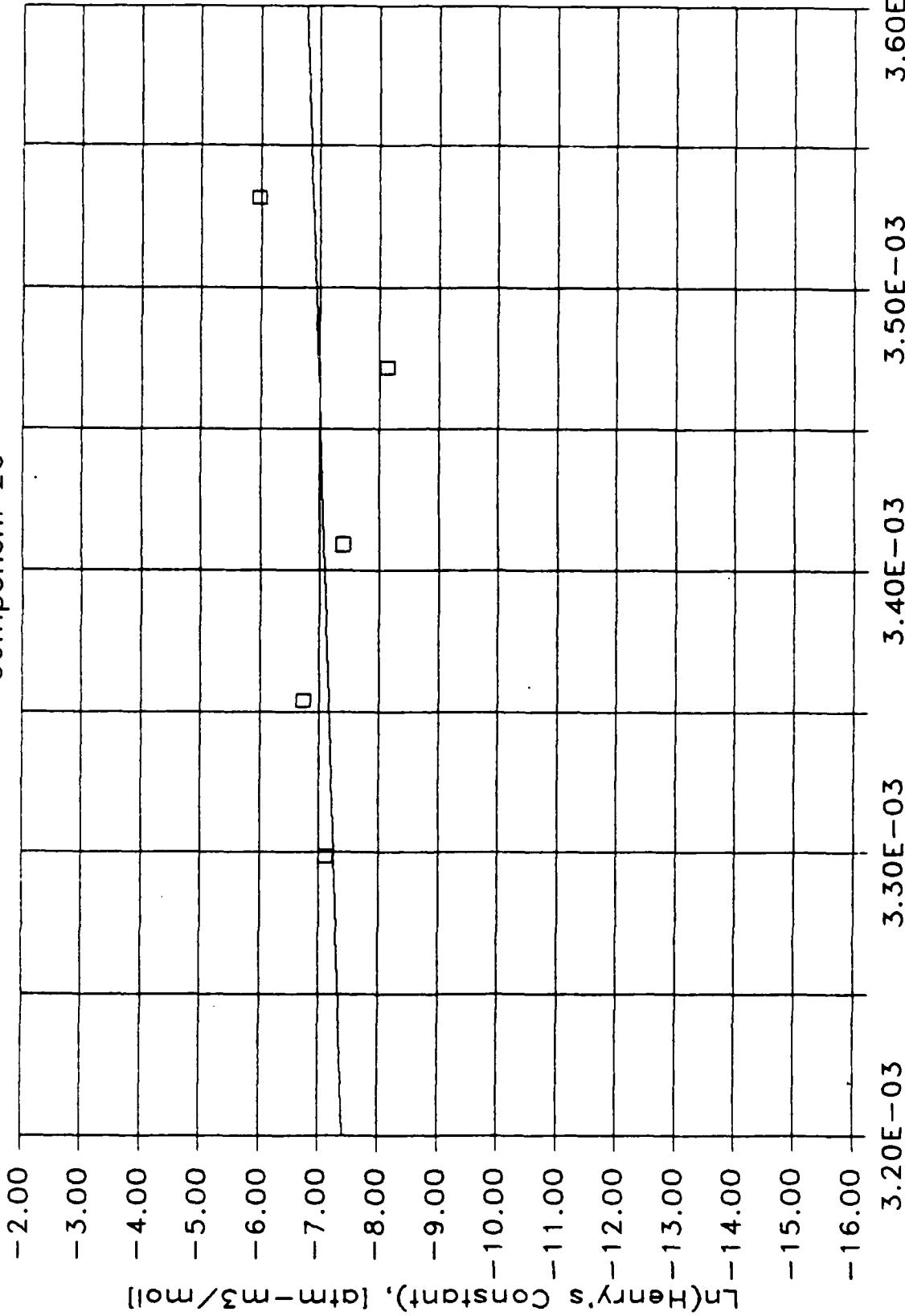
SLOPE = 1.6E+03

Y-INTERCEPT = -1.3E+01

R-SQUARED = 0.0339

TEMPERATURE REGRESSION PLOT

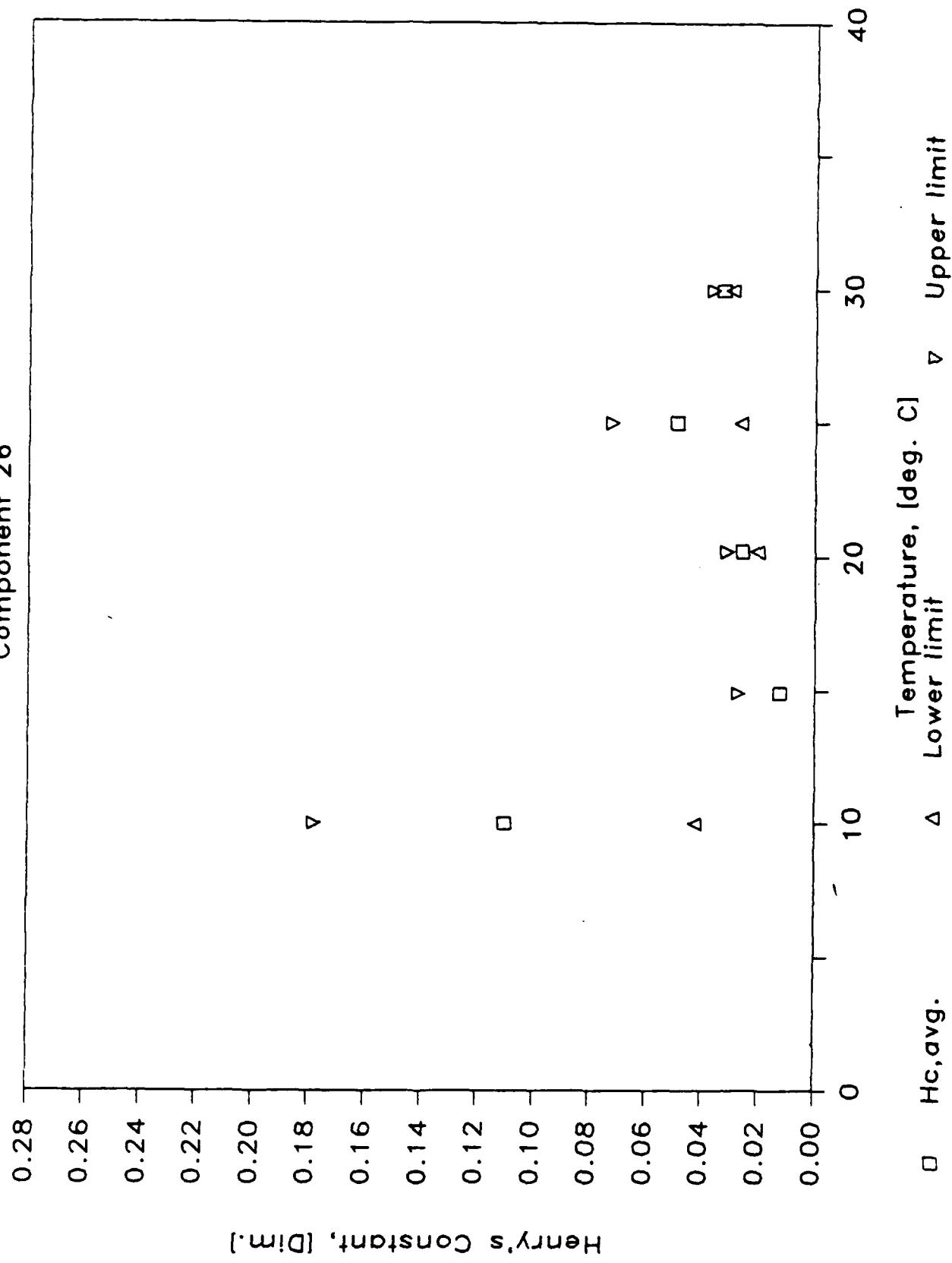
Component 26



□ Experimental data
— Reciprocal Temperature, [1/K]

Regr: r-sq. = 0.0339

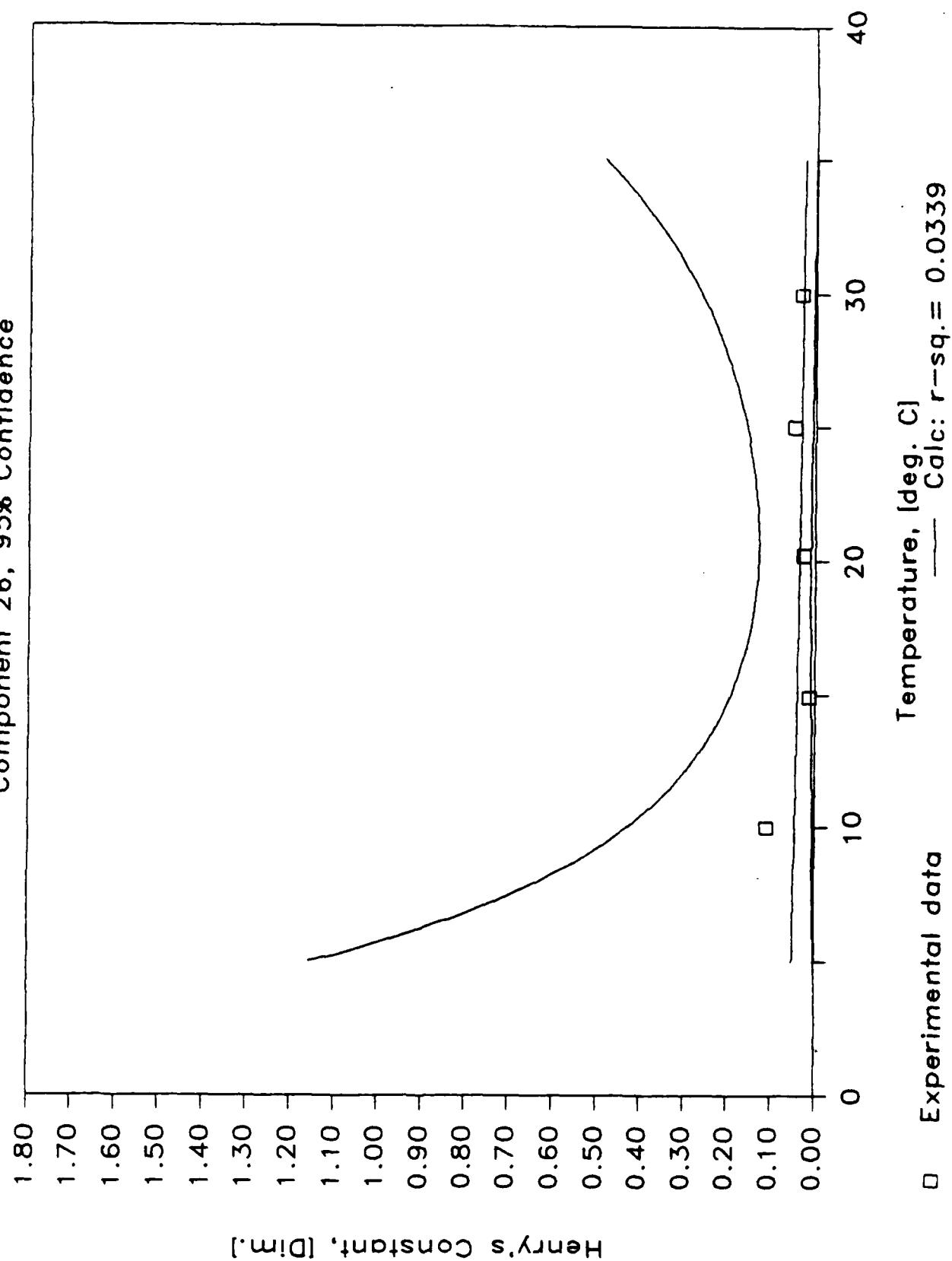
95% CONFIDENCE TEST
Component 26



REGRESSION CONFIDENCE TEST

Component 26, 95% Confidence

219



06-Nov-86

Results Summary for Component 27

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	12	No. 1	No. 2	5	No. 1	No. 2
REPLICATE -->						
Group No.		7		7		7
Component ID		27		27		27
Temperature (C)		10		14.9		20.2
Low Vol (ml)		30		30		30
High Vol (ml)		210		210		210
System Vol (ml)		250		250		250
H, avg: atm-m3/mol	0.1399	1.0E-25		0.0724	1.0E-25	0.0880
H, avg: atm-m3/mol	180.5			95.0		106.9
H, avg: atm-m3/mol	3.25E-03	1		1.71E-03	1	1.93E-03
H, avg: kPa-m3/mol	0.3294			0.1734		0.1952
COV, r [std/mean]	35.68			9.98		10.94
COV, both replic.	_____			_____		_____
Observation: (1)	0.1736			0.0798		0.0868
[atm-m3/mol] (2)	0.1914			0.0772		0.0883
(3)	0.0910			0.0675		0.0718
(4)	0.1038			0.0658		0.0732
Injection: (1)	294410			250860		312960
[Peak Area] (2)	219290			237090		291860
(3)	936760			1124600		1356900
(4)	888750			1137600		1348100

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		13		5	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		7		7	
Component ID		27		27	
Temperature (C)		25		39	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.0608	1.0E-25	0.1072	1.0E-25
H, avg: atm-mol/mol		93.5		148.0	
H, avg: atm-m3/mol		1.68E-03	1	2.67E-03	1
H, avg: kPa-m3/mol		0.1706		0.2702	
COV, r [std/mean]		5.80		10.34	
COV, both replic.		_____		_____	
Observation: (1)		0.0713		0.1150	
[atm-m3/m3] (2)		0.0730		0.1183	
(3)		0.0646		0.0962	
(4)		0.0663		0.0993	
Injection: (1)		388130		591170	
[Peak Area] (2)		376150		548890	
(3)		1808500		2294500	
(4)		1793800		2265500	

Temperature Regression Parameters:

OF POINTS = 5

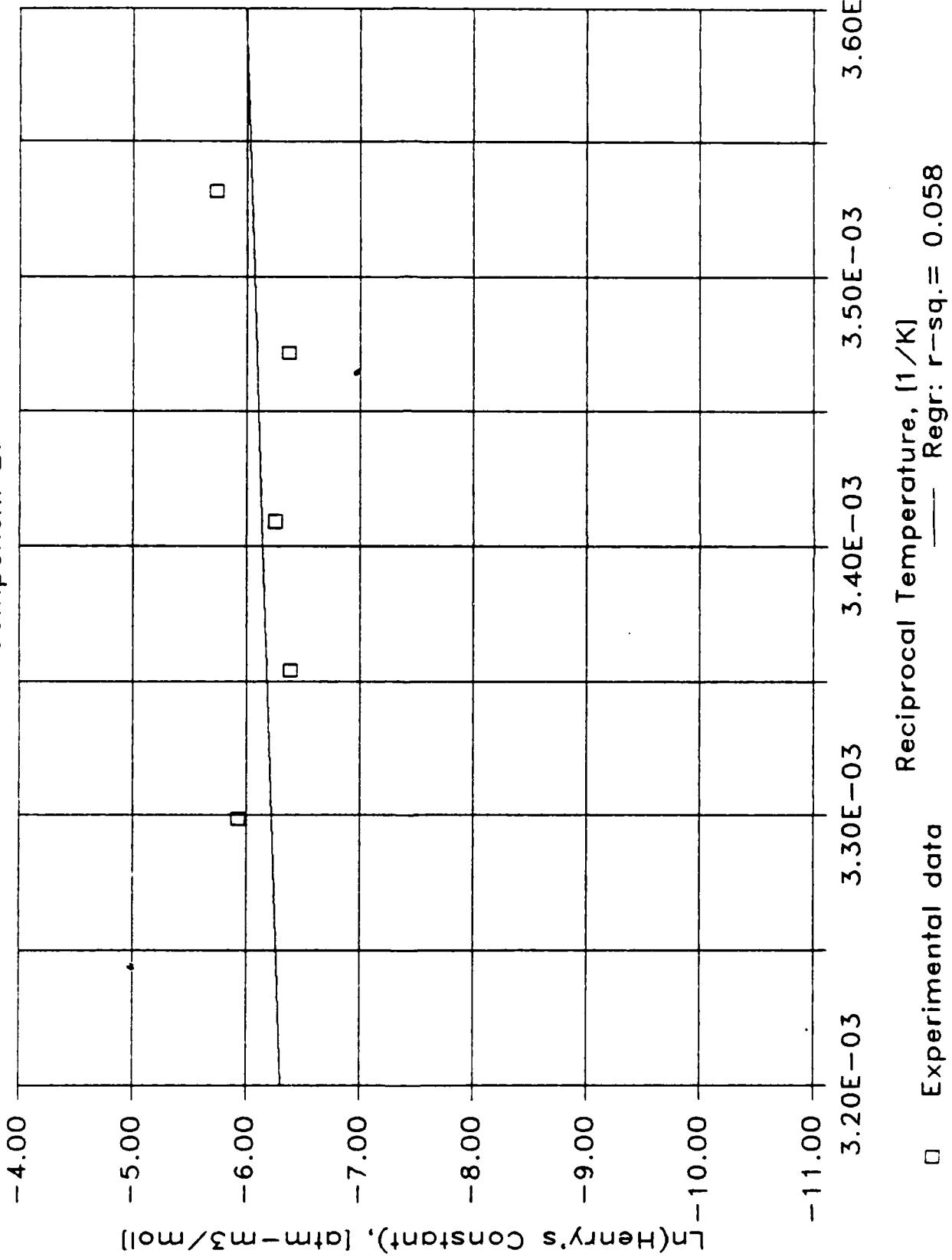
SLOPE = 7.6E+02

Y-INTERCEPT = -8.7E+00

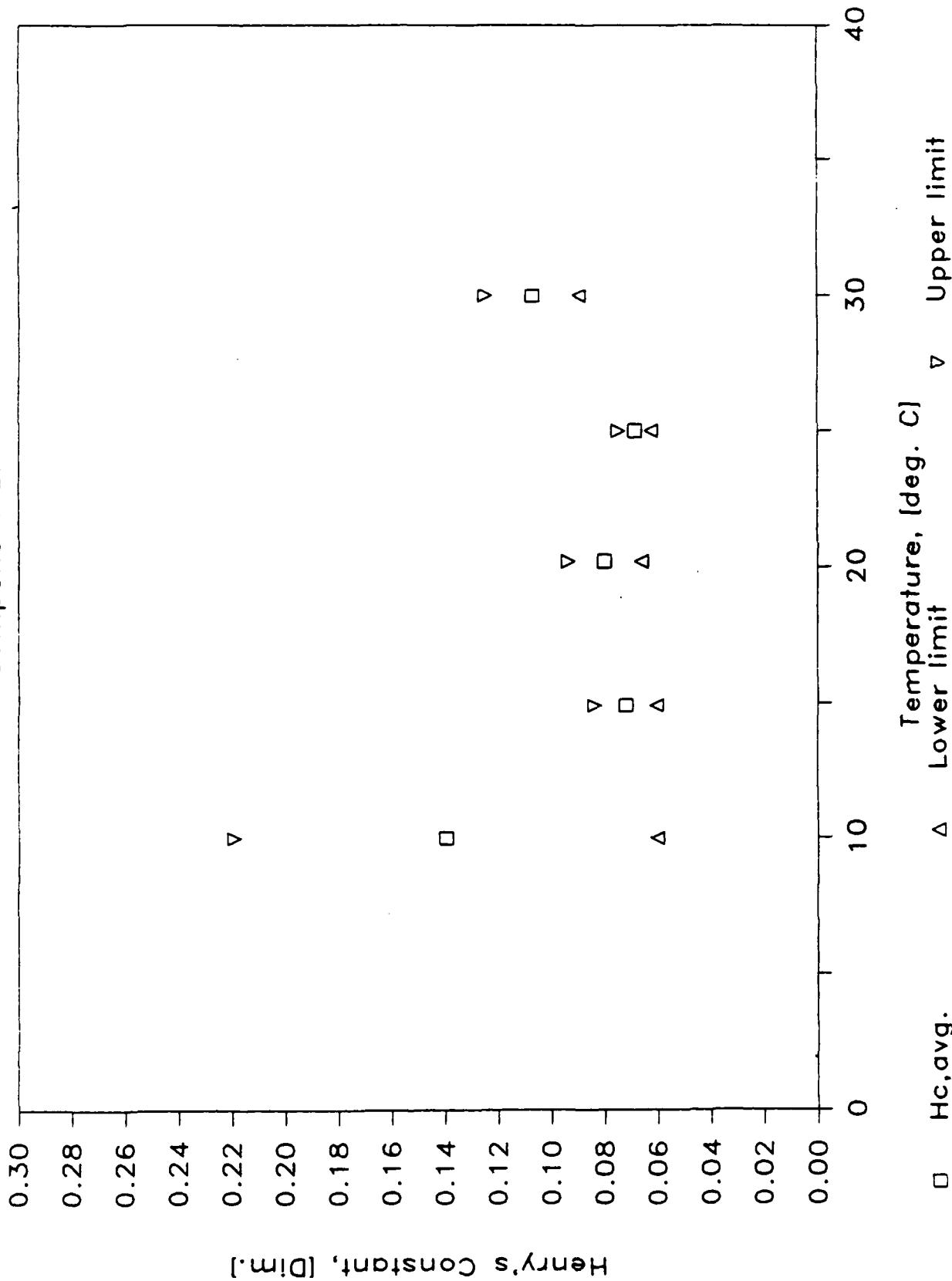
R-SQUARED = 0.0589

TEMPERATURE REGRESSION PLOT

Component 2⁷



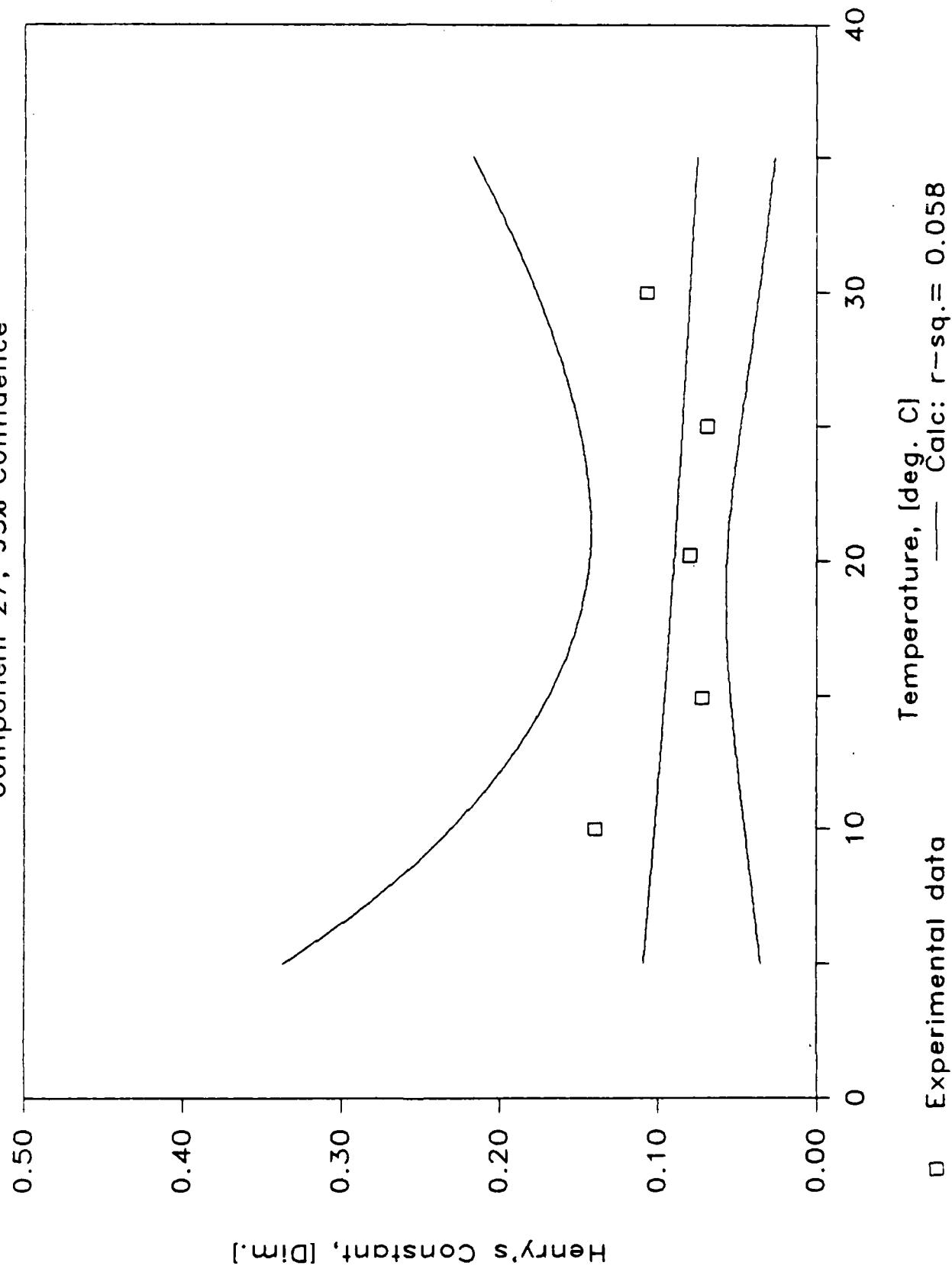
95% CONFIDENCE TEST
Component 27



REGRESSION CONFIDENCE TEST

Component 27, 95% Confidence

224



11-Nov-86

Results Summary for Component 127

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	6	No. 1 No. 2	6	No. 1 No. 2	7	No. 1 No. 2
REPLICATE →						
Group No.		1		1		1
Component ID		127		127		127
Temperature (C)		10.1		15		20
Low Vol (ml)		30		30		30
High Vol (ml)		210		210		210
System Vol (ml)		250		250		250
H, avg: atm=m3/m3		0.0321 1.0E-25		0.0445 1.0E-25		0.0563 1.0E-25
H, avg: atm=mol/mol		41.5		58.4		75.2
H, avg: atm=m3/mol		7.47E-04 1		1.05E-03 1		1.35E-03 1
H, avg: kPa=m3/mol		0.0757		0.1066		0.1373
COV, r [std/mean]		38.85		30.24		17.79
COV, both replic.		_____		_____		_____
Observation:	(1)	0.0343		0.0568		0.0656
[atm=m3/m3]	(2)	0.0476		0.0555		0.0643
	(3)	0.0174		0.0334		0.0482
	(4)	0.0293		0.0323		0.0471
Injection:	(1)	385740		338690		411480
[Peak Area]	(2)	348690		299060		377340
	(3)	2171800		1692200		1969100
	(4)	2020000		1703100		1981100

11-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		7		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		1		1	
Component ID		127		127	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H _a avg: atm-m ³ /mol		0.0763	1.0E-25	0.1078	1.0E-25
H _a avg: atm-mol/mol		103.6		148.8	
H _a avg: atm-m ³ /mol		1.87E-03	1	2.68E-03	1
H _a avg: kPa-m ³ /mol		0.1891		0.2717	
COV, r [std/mean]		10.03		3.26	
COV, both replic.		_____		_____	
Observation: (1)		0.0817		0.1073	
[atm-m ³ /mol]	(2)	0.0839		0.1035	
(3)		0.0687		0.1121	
(4)		0.0708		0.1082	
Injection:	(1)	547240		989510	
[Peak Area]	(2)	515850		1007900	
(3)		2432400		3954900	
(4)		2409100		4014900	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

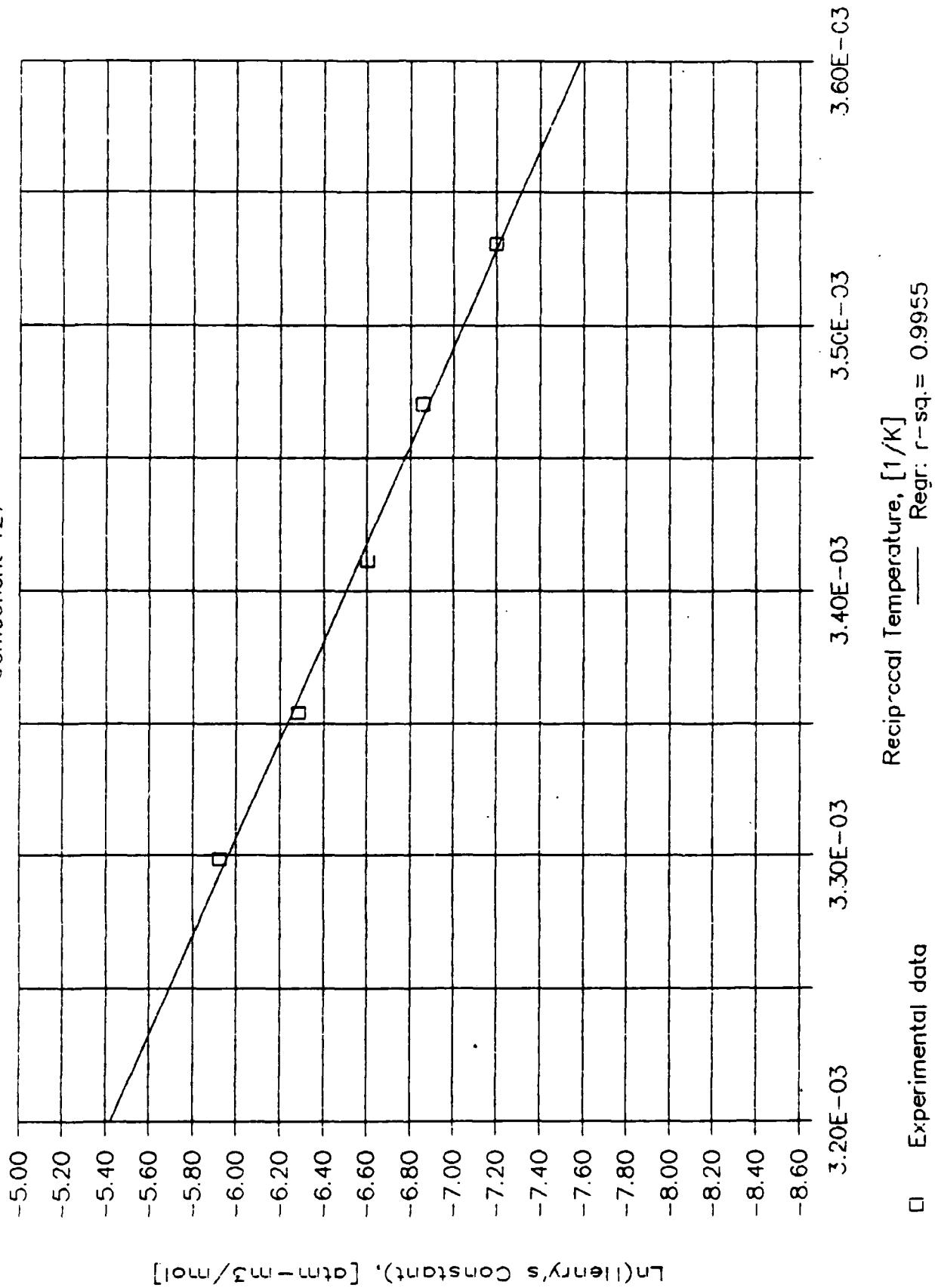
SLOPE = -5.4E+03

Y-INTERCEPT = 1.2E+01

R-SQUARED = 0.9955

TEMPERATURE REGRESSION PLOT

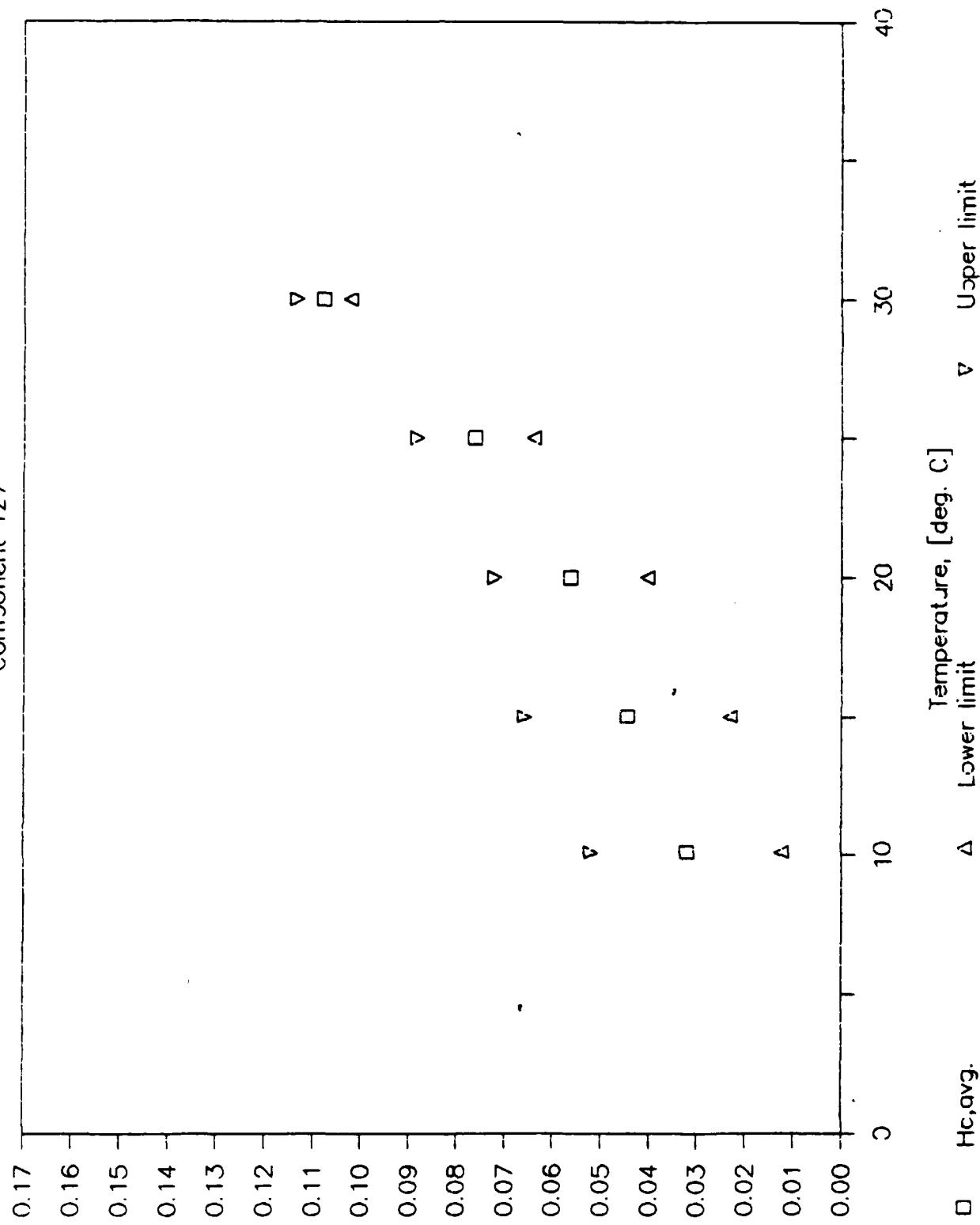
Component 127



95% CONFIDENCE TEST

Component 127

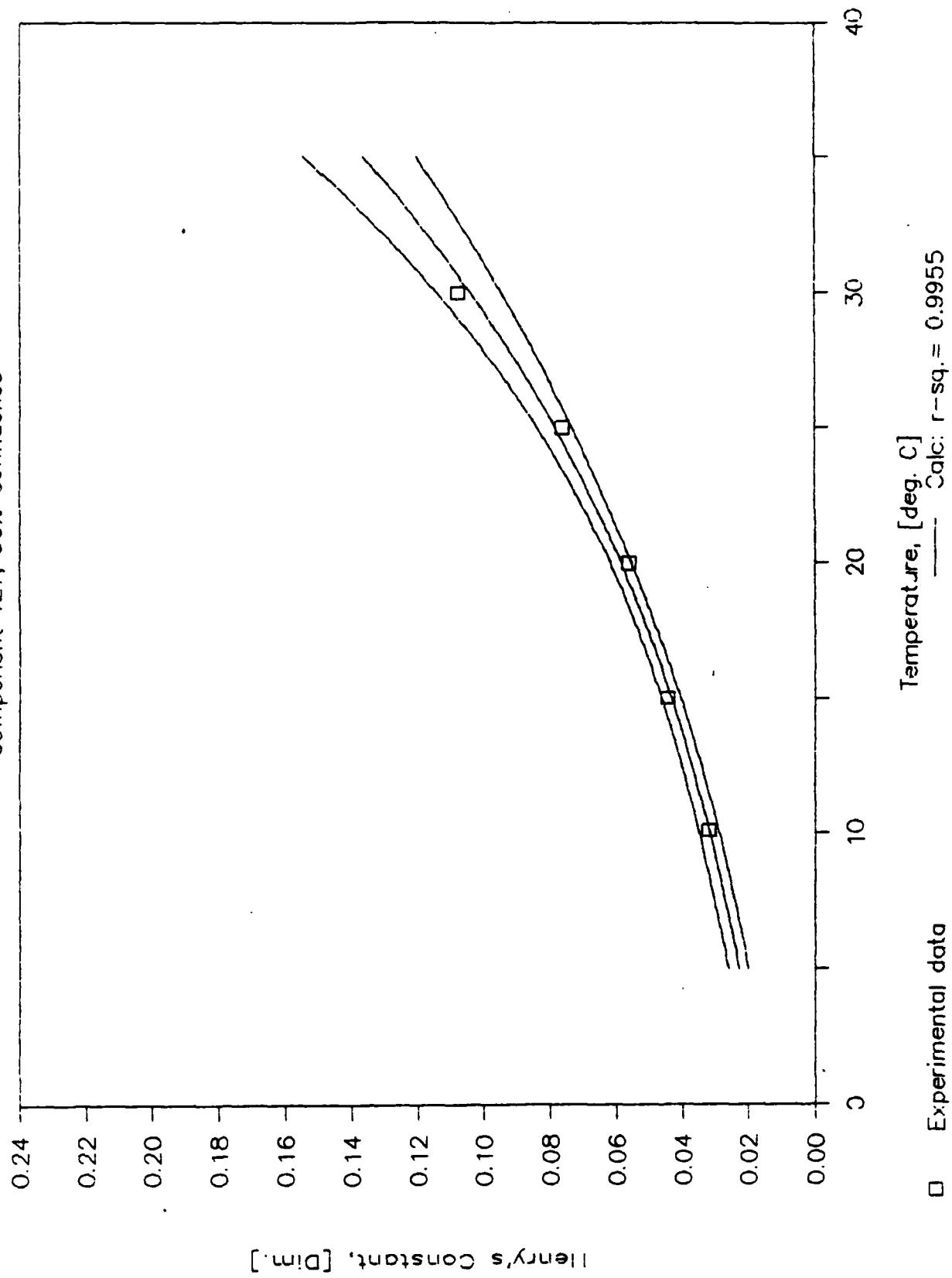
225



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 127, 95% Confidence



06-Nov-86

Results Summary for Component 28

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		16		9		10	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		7		7		7	
Component ID		28		28		28	
Temperature (C)		10		14.9		20.2	
Low Vol (ml)		30		30		30	
High Vol (ml)		210		210		210	
System Vol (ml)		250		250		250	
H ₄ avg: atm-m ³ /m ³		3.8126	1.0E-25	3.5411	1.0E-25	4.3860	1.0E-25
H ₄ avg: atm-mol/mol		3885.4		4646.0		5860.3	
H ₄ avg: atm-m ³ /mol		7.00E-02	1	8.37E-02	1	1.06E-01	1
H ₄ avg: kPa-m ³ /mol		7.0927		8.4812		10.6979	
COV, r [std/mean]		6.96		7.74		4.97	
COV, both replic.		_____		_____		_____	
Observation: (1)		2.9477		3.5045		4.6384	
[atm-m ³ /m ³] (2)		3.2691		3.8863		4.4800	
(3)		2.7690		3.2174		4.2835	
(4)		3.0646		3.5563		4.1419	
Injection: (1)		392540		348300		376960	
[Peak Area] (2)		378040		331710		361930	
(3)		189710		152270		141940	
(4)		178540		143830		144460	

86-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	17	9	No. 1	No. 2
REPLICATE →				
Group No.	7		7	
Component ID	28		28	
Temperature (C)	25		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H _a avg: atm-m ³ /m ³	4.7742	1.0E-25	7.9859	1.0E-25
H _a avg: atm-mol/mol	6483.5		11026.9	
H _a avg: atm-m ³ /mol	1.17E-01	1	1.99E-01	1
H _a avg: kPa-m ³ /mol	11.8355		20.1293	
COV, r [std/mean]	6.79		13.94	
COV, both replic.	—		—	
Observation: (1)	4.4337		6.8838	
[atm-m ³ /m ³] (2)	4.9615		7.2016	
(3)	4.5744		8.6974	
(4)	5.1273		9.1614	
Injection: (1)	504230		542490	
[Peak Area] (2)	512310		593900	
(3)	194260		170490	
(4)	183640		167370	

Temperature Regression Parameters:

OF POINTS = 5

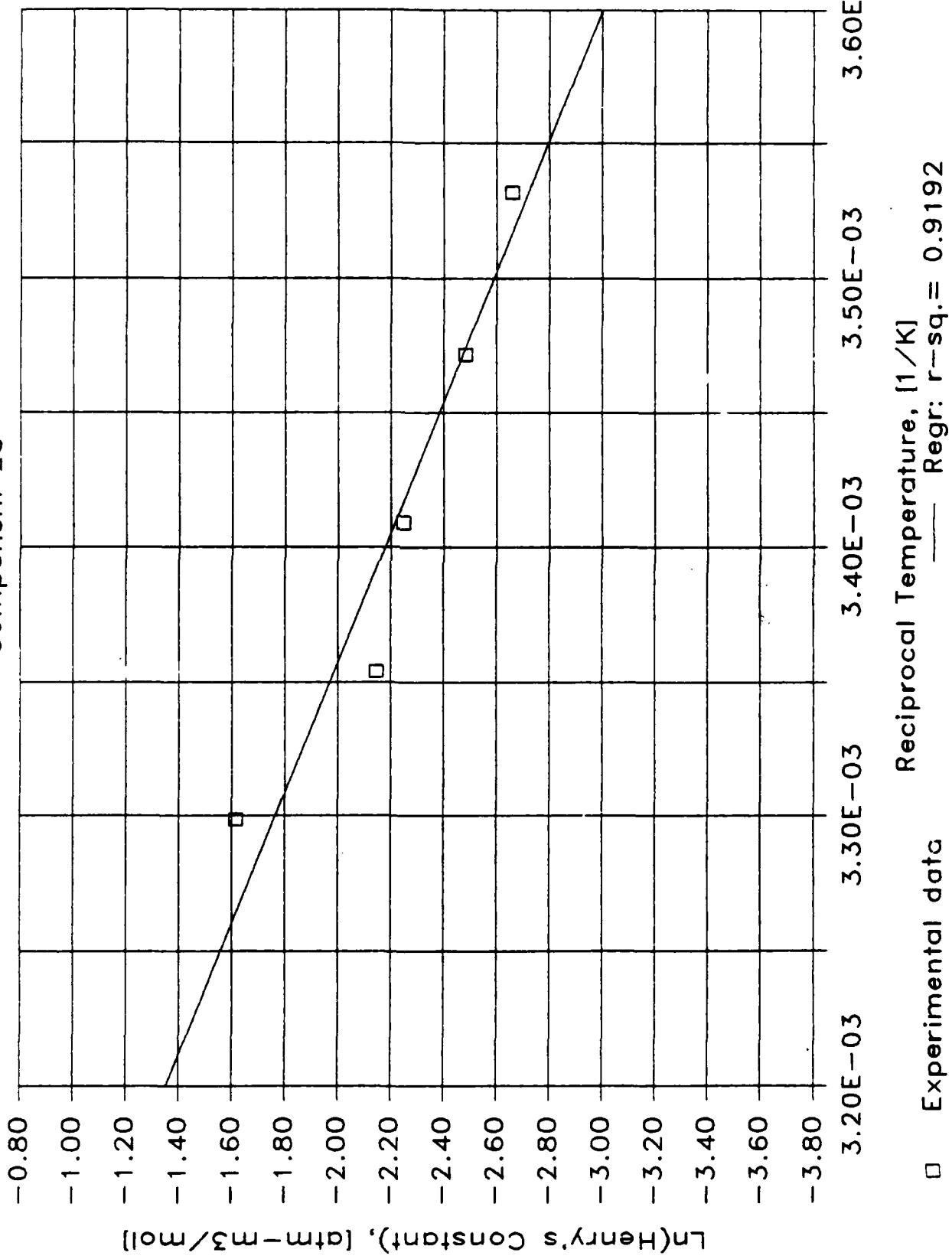
SLOPE = -4.1E+03

Y-INTERCEPT = 1.2E+01

R-SQUARED = 0.9192

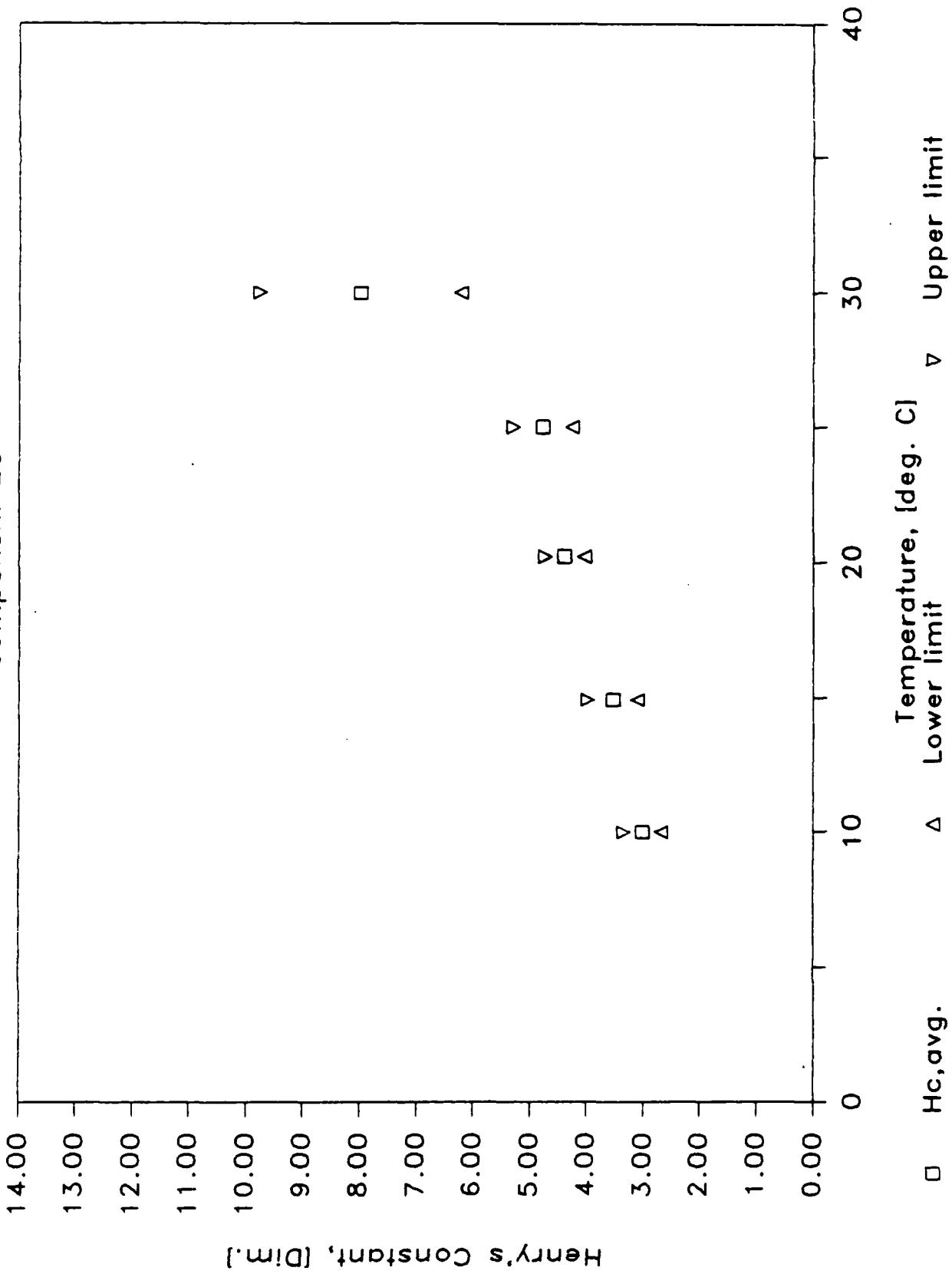
TEMPERATURE REGRESSION PLOT

Component 28



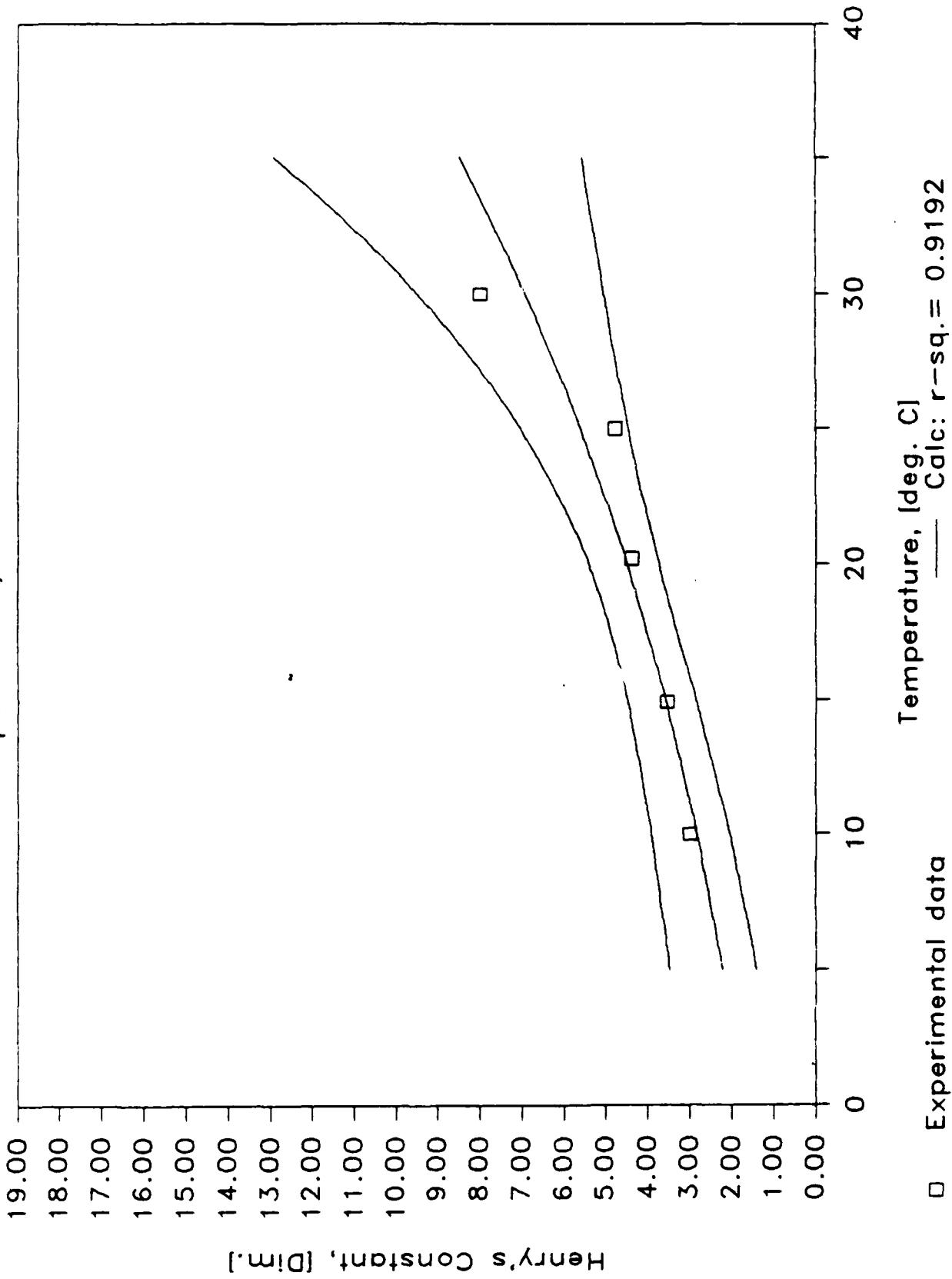
95% CONFIDENCE TEST
Component 28

233



REGRESSION CONFIDENCE TEST

Component 28, 95% Confidence



		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		57		74		5	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		15		15		15	
Component ID		128		128		128	
Temperature (C)		10		15.2		19.9	
Low Vol (ml)		30		30		30	
High Vol (ml)		210		210		210	
System Vol (ml)		250		250		250	
H ₄ avg: atm-m3/m3		2.8119	1.0E-25	3.2727	1.0E-25	4.0582	1.0E-25
H ₄ avg: atm-mol/mol		3626.5		4298.3		5416.9	
H ₄ avg: atm-m3/mol		6.53E-02	1	7.74E-02	1	9.76E-02	1
H ₄ avg: kPa-m3/mol		6.6201		7.8464		9.8884	
COV, r [std/mmean]		17.41		9.34		5.76	
COV, both replic.		_____		_____		_____	
Observation: (1)		2.3697		3.0019		3.9925	
[atm-m3/m3] (2)		2.4072		3.5293		4.3445	
(3)		3.2075		3.0145		3.7848	
(4)		3.2631		3.5450		4.1110	
Injections: (1)		272660		355170		292260	
[Peak Area] (2)		327770		356050		283940	
(3)		150730		169800		118950	
(4)		149240		154660		113780	

RUN Number →	Temperature 4		Temperature 5	
	75	58	No. 1	No. 2
REPLICATE →	No. 1	No. 2	No. 1	No. 2
Group No.	15		15	
Component ID	128		128	
Temperature (C)	25.15		30	
Low Vol (ml)	30		30	
High Vol (ml)	210		210	
System Vol (ml)	250		250	
H ₄ avg: atm-m ³ /m ³	5.3682	1.0E-25	9.1613	1.0E-25
H ₄ avg: atm-mol/mol	7293.9		12650.0	
H ₄ avg: atm-m ³ /mol	1.31E-01	1	2.28E-01	1
H ₄ avg: kPa-m ³ /mol	13.3147		23.0922	
COV, r [std/mean]	3.19		27.78	
COV, both replic.	_____		_____	
Observation: (1)	5.3430		8.7157	
[atm-m ³ /m ³] (2)	5.5796		6.4985	
(3)	5.1628		12.6278	
(4)	5.3876		8.8034	
Injection: (1)	462700		494020	
[Peak Area] (2)	455230		536470	
(3)	162640		141710	
(4)	159390		159050	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

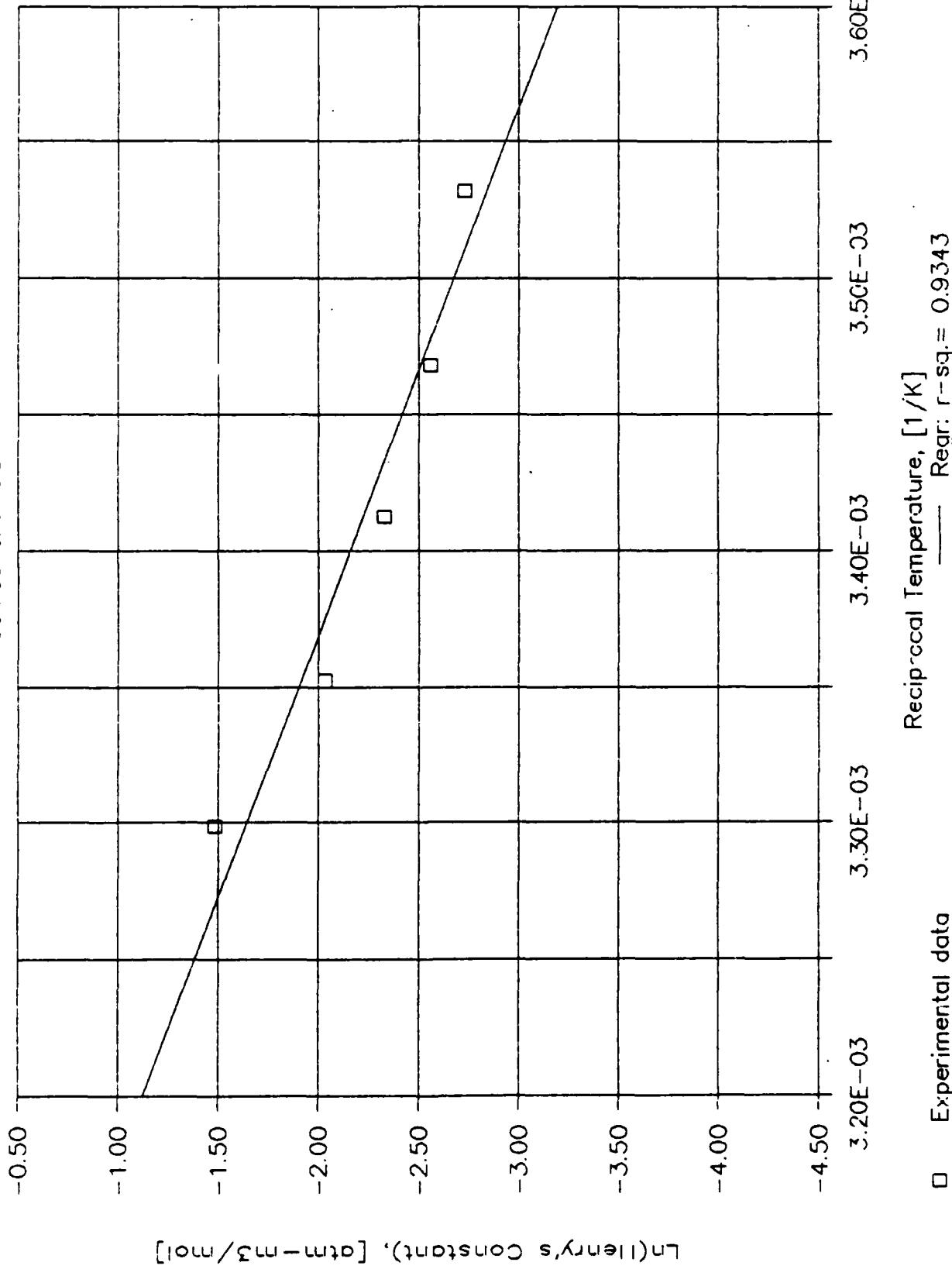
SLOPE = -5.2E+03

Y-INTERCEPT = 1.5E+01

R-SQUARED = 0.9343

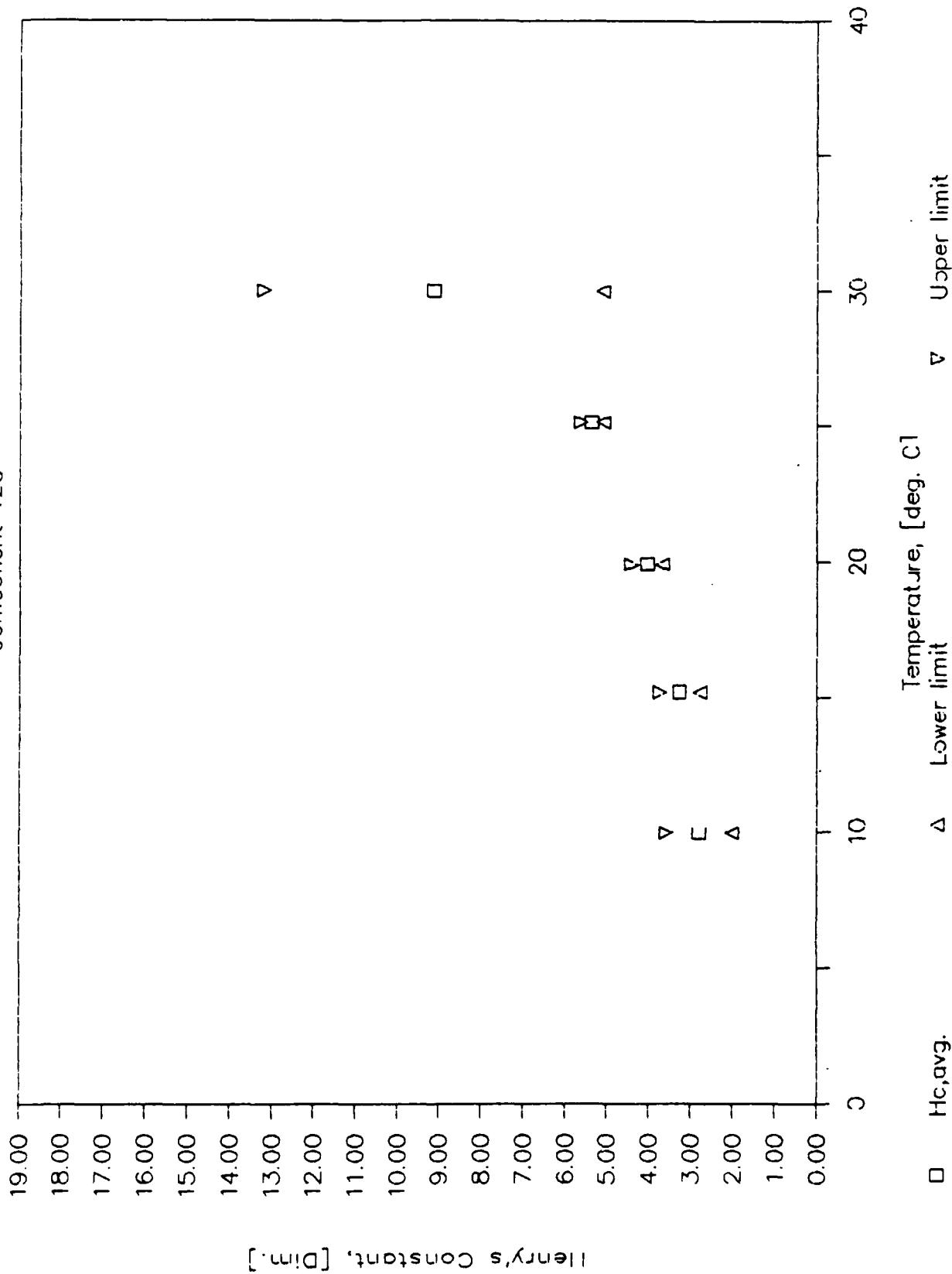
TEMPERATURE REGRESSION PLOT

Component 128



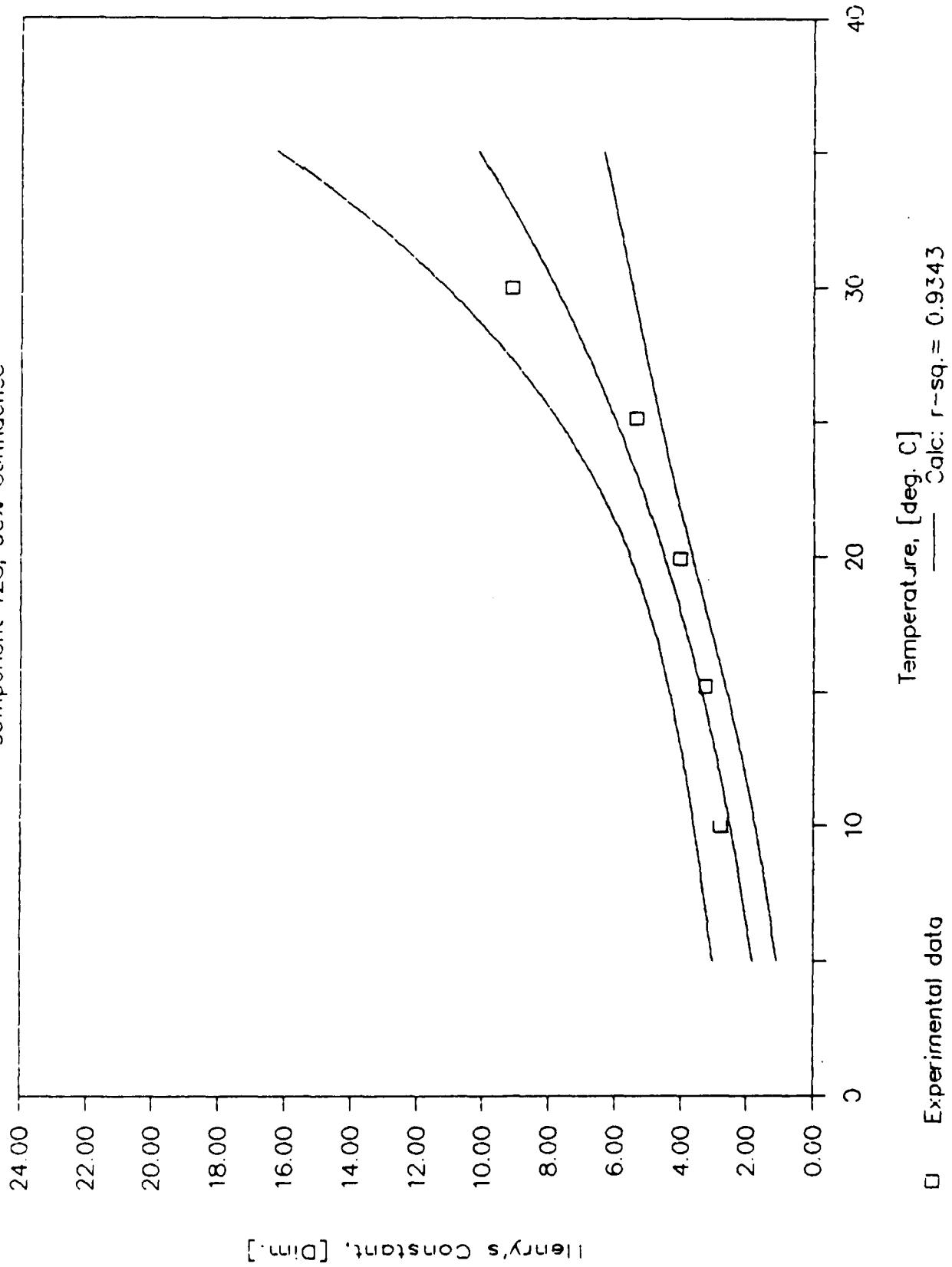
95% CONFIDENCE TEST
Component 128

238



REGRESSION CONFIDENCE TEST

Component 128, 95% Confidence



06-Nov-86

Results Summary for Component 38

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE →						
Group No.	8		8		8	
Component ID	38		38		38	
Temperature (C)	10		15		20.2	
Low Vol (ml)	20		20		20	
High Vol (ml)	200		200		200	
System Vol (ml)	250		250		250	
H, avg: atm-m3/m3	0.4585	1.0E-25	0.5583	1.0E-25	0.6020	1.0E-25
H, avg: atm-mol/mol	581.0		722.3		804.3	
H, avg: atm-m3/mol	1.05E-02	1	1.38E-02	1	1.45E-02	1
H, avg: kPa-m3/mol	1.0606		1.3185		1.4683	
COV, r [std/mean]	3.89		6.31		9.12	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.4365		0.5365		0.6476	
[atm-m3/m3] (2)	0.4342		0.5914		0.5529	
(3)	0.4669		0.5105		0.6513	
(4)	0.4644		0.5628		0.5560	
Injection: (1)	933510		1043000		1135300	
[Peak Area] (2)	980890		1085300		1148100	
(3)	1719900		1649800		1561500	
(4)	1726600		1534600		1756200	

86-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		15		14	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		8		8	
Component ID		39		39	
Temperature (C)		25		39	
Low Vol (ml)		20		20	
High Vol (ml)		200		200	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.9061	1.0E-25	0.7089	1.0E-25
H, avg: atm-mol/mol		1230.5		978.8	
H, avg: atm-m3/mol		2.22E-02	1	1.76E-02	1
H, avg: kPa-m3/mol		2.2462		1.7869	
COV, r [std/mean]		6.18		19.09	
COV, both replic.		—		—	
Observation: (1)		0.9572		0.5666	
[atm-m3/m3] (2)		0.9517		0.6295	
(3)		0.8601		0.7761	
(4)		0.8552		0.8634	
Injection: (1)		1864900		1051500	
[Peak Area] (2)		1725200		1327700	
(3)		1924700		1597300	
(4)		1932700		1477000	

Temperature Regression Parameters:

OF POINTS = 5

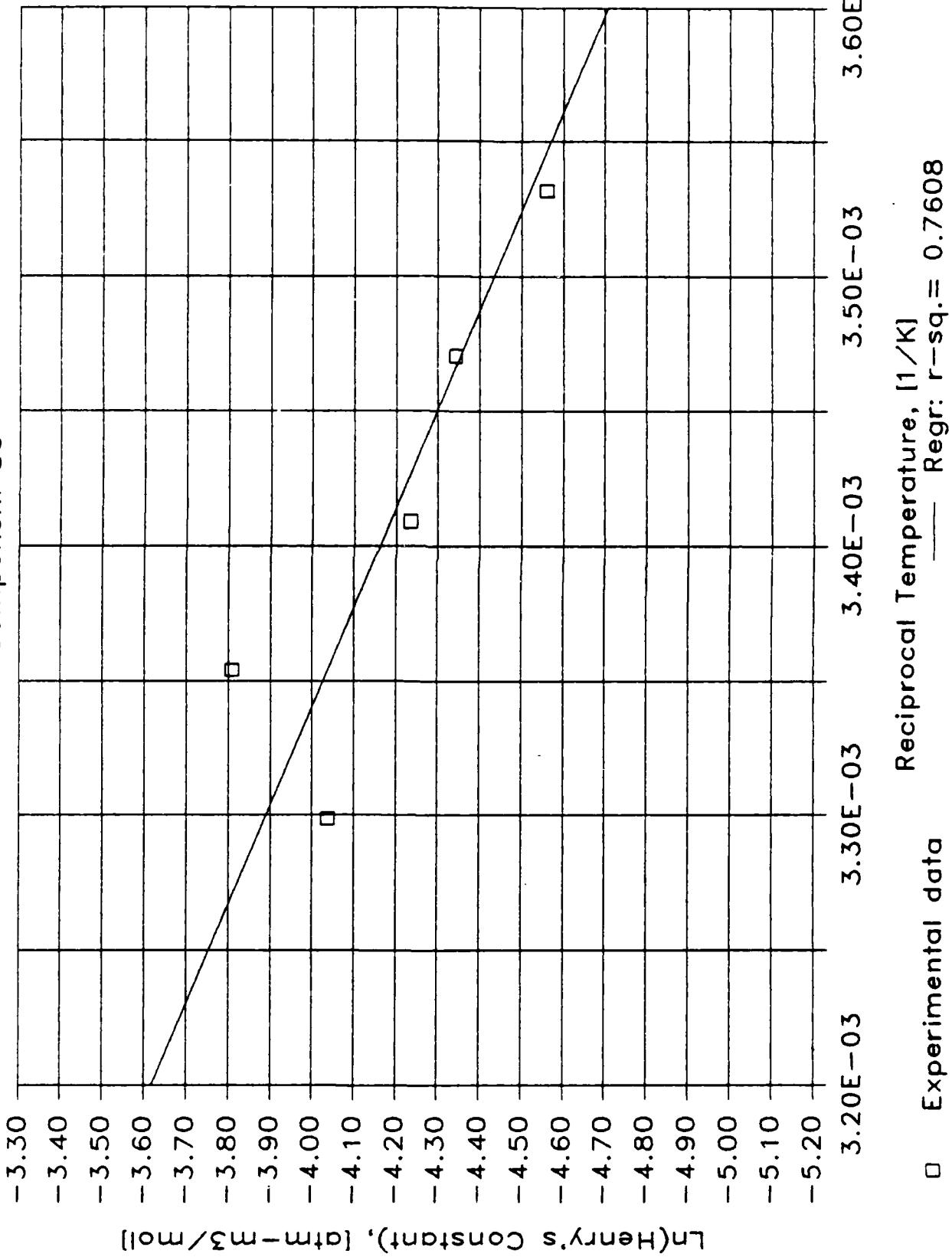
SLOPE = -2.7E+03

Y-INTERCEPT = 5.1E+00

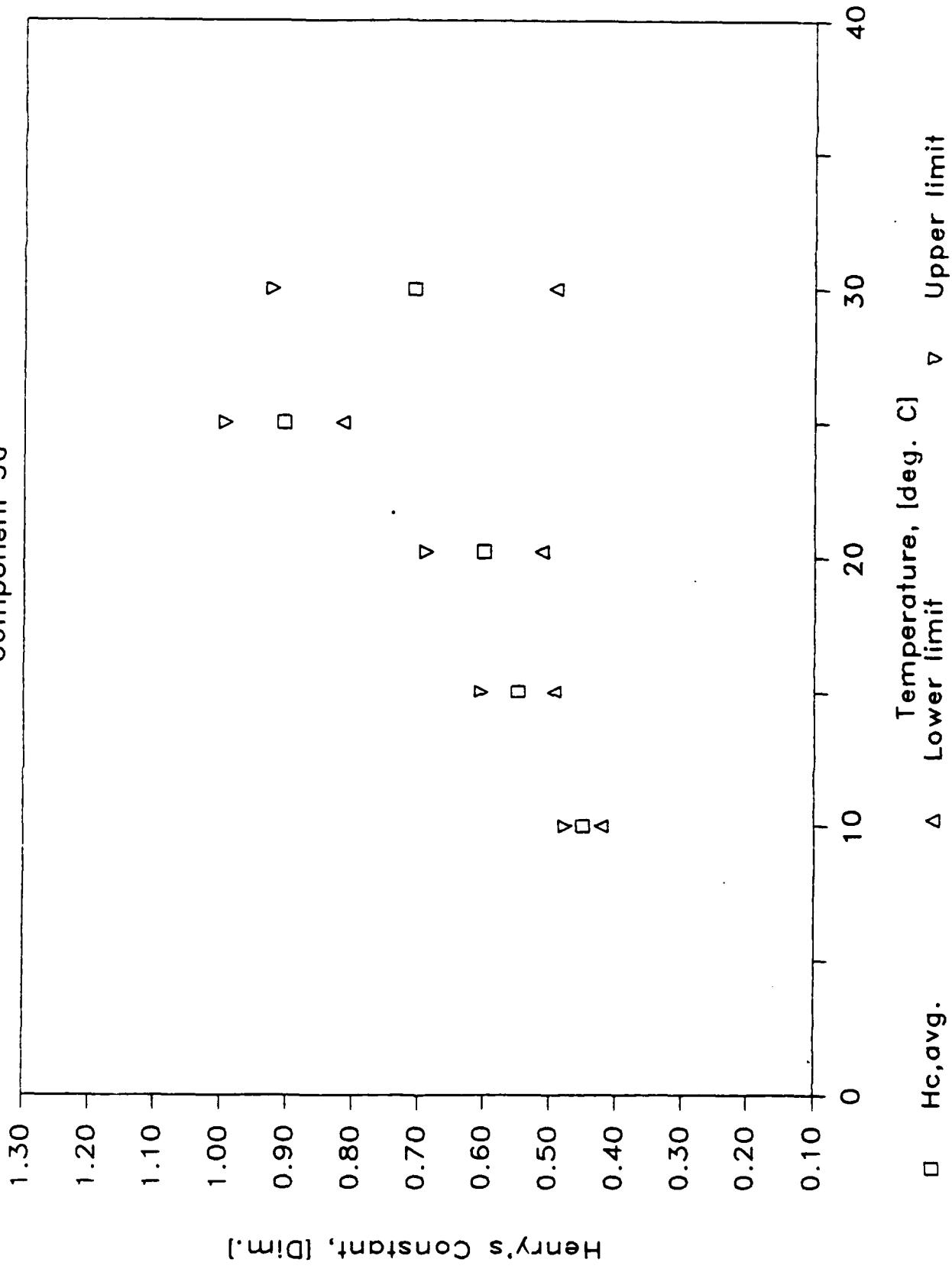
R-SQUARED = 0.7688

TEMPERATURE REGRESSION PLOT

Component 30



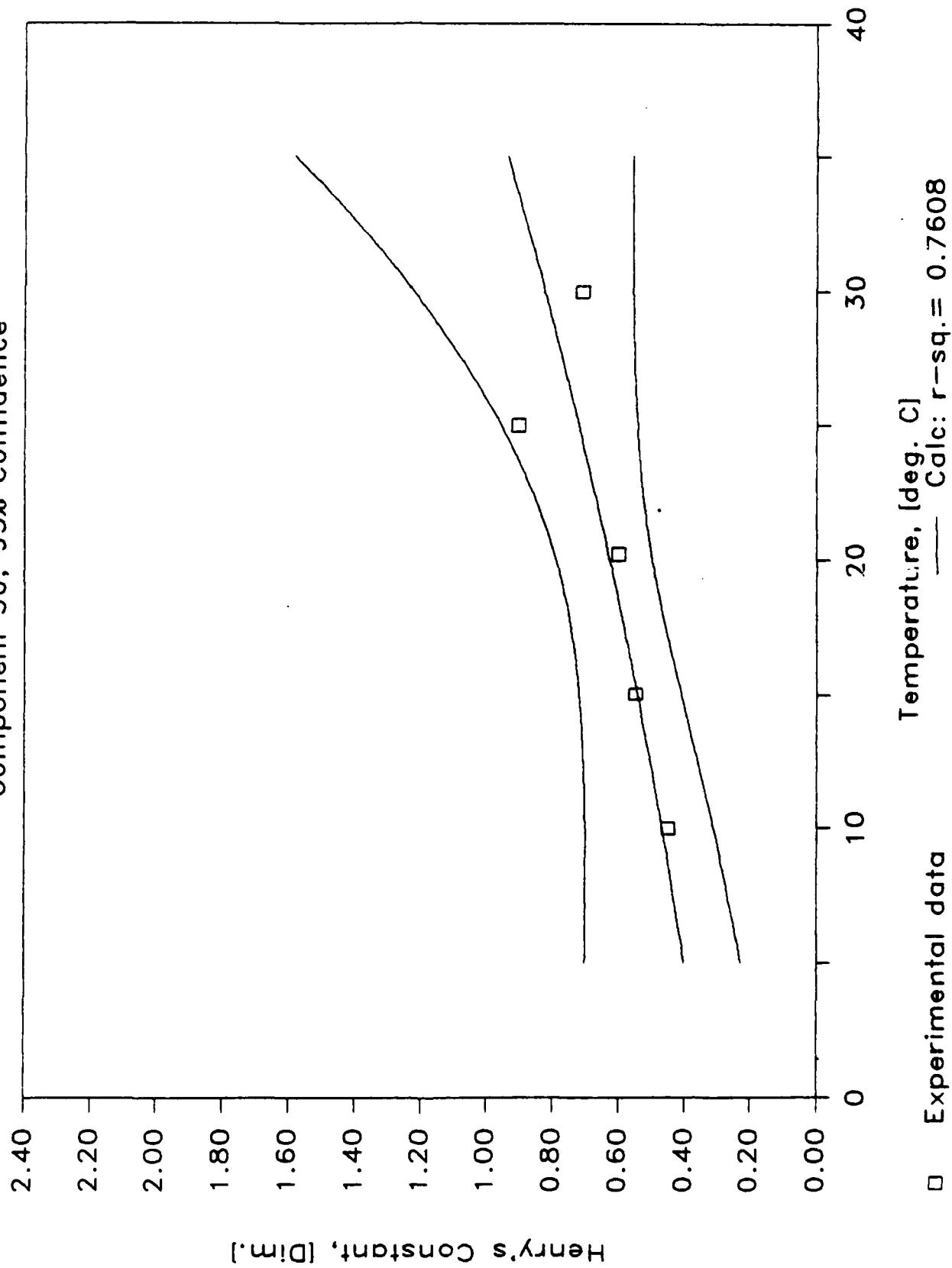
95% CONFIDENCE TEST
Component 30



REGRESSION CONFIDENCE TEST

Component 30, 95% Confidence

244



04-Nov-86

Results Summary for Component 130

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	16		16		16	
Component ID	130		130		130	
Temperature (C)	10		15		20.1	
Low Vol (ml)	20		20		20	
High Vol (ml)	200		200		200	
System Vol (ml)	250		250		250	
H, avg: atm=m3/m3	0.6456	1.0E-25	0.7103	1.0E-25	0.9035	1.0E-25
H, avg: atm=mol/mol	832.7		932.2		1206.8	
H, avg: atm=m3/mol	1.50E-02	1	1.68E-02	1	2.17E-02	1
H, avg: kPa-m3/mol	1.5200		1.7017		2.2030	
COV, r [std/mean]	1.27		1.63		0.62	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.6521		0.7245		0.9061	
[atm=m3/m3] (2)	0.6379		0.7104		0.9098	
(3)	0.6534		0.7099		0.8972	
(4)	0.6392		0.6962		0.9008	
Injection: (1)	1372200		1544100		1765200	
[Peak Area] (2)	1374300		1521100		1752500	
(3)	1877800		1954400		1895800	
(4)	1908700		1982900		1890200	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		3		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		16		16	
Component ID		130		130	
Temperature (C)		25.1		30	
Low Vol (ml)		20		20	
High Vol (ml)		200		200	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		1.0821	1.0E-25	1.1273	1.0E-25
H, avg: atm-mol/mol		1470.0		1556.5	
H, avg: atm-m3/mol		2.65E-02	1	2.80E-02	1
H, avg: kPa-m3/mol		2.6835		2.8414	
COV, r [std/mean]		1.24		2.97	
COV, both replic.		_____		_____	
Observation: (1)		1.0896		1.1408	
[atm-m3/m3] (2)		1.0967		1.1661	
(3)		1.0676		1.0891	
(4)		1.0746		1.1131	
Injection: (1)		2142000		2314200	
[Peak Area] (2)		2111100		2239200	
(3)		2014400		2106500	
(4)		2005000		2074100	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

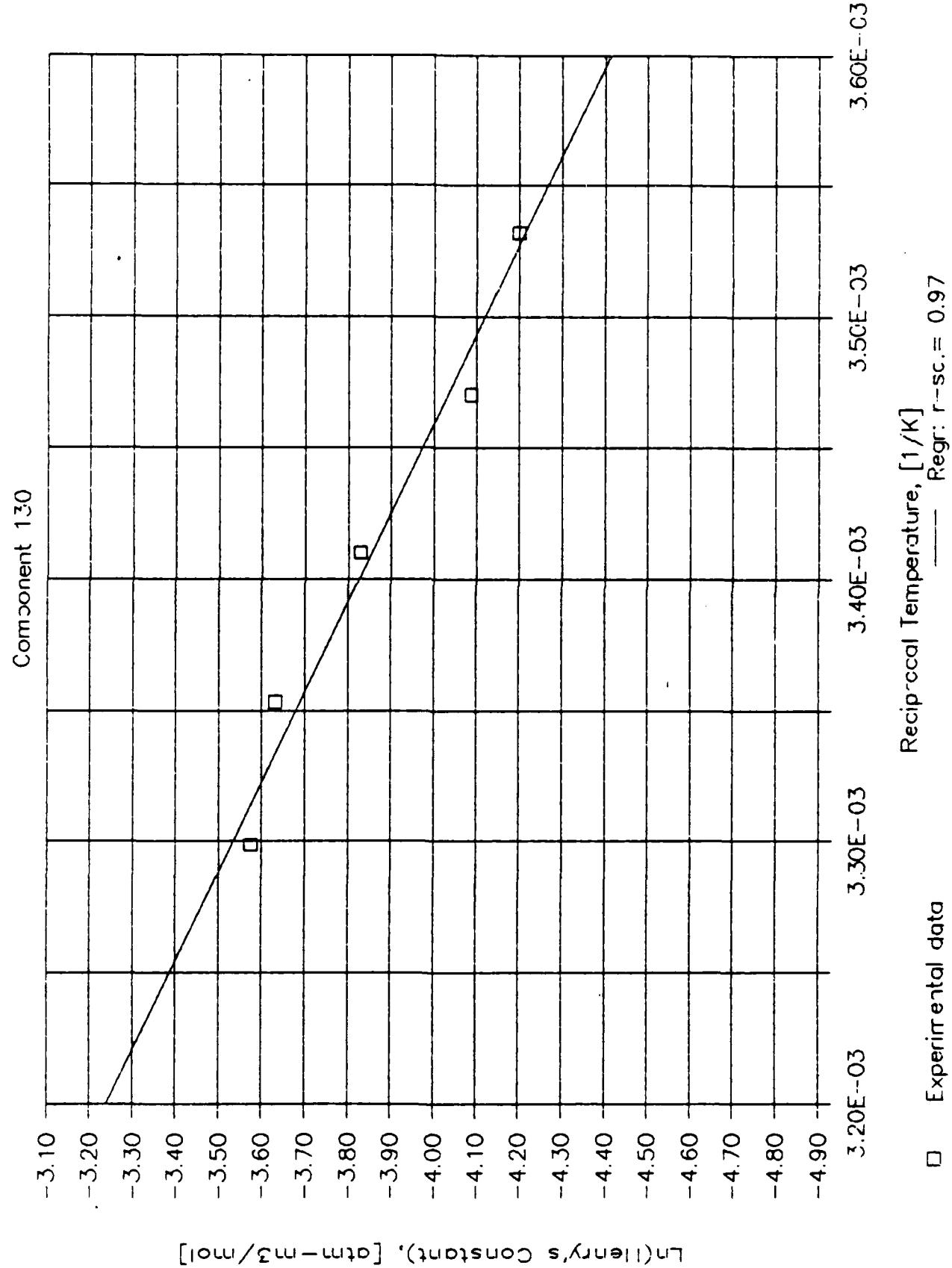
OF POINTS = 5

SLOPE = -2.9E+03

Y-INTERCEPT = 6.1E+00

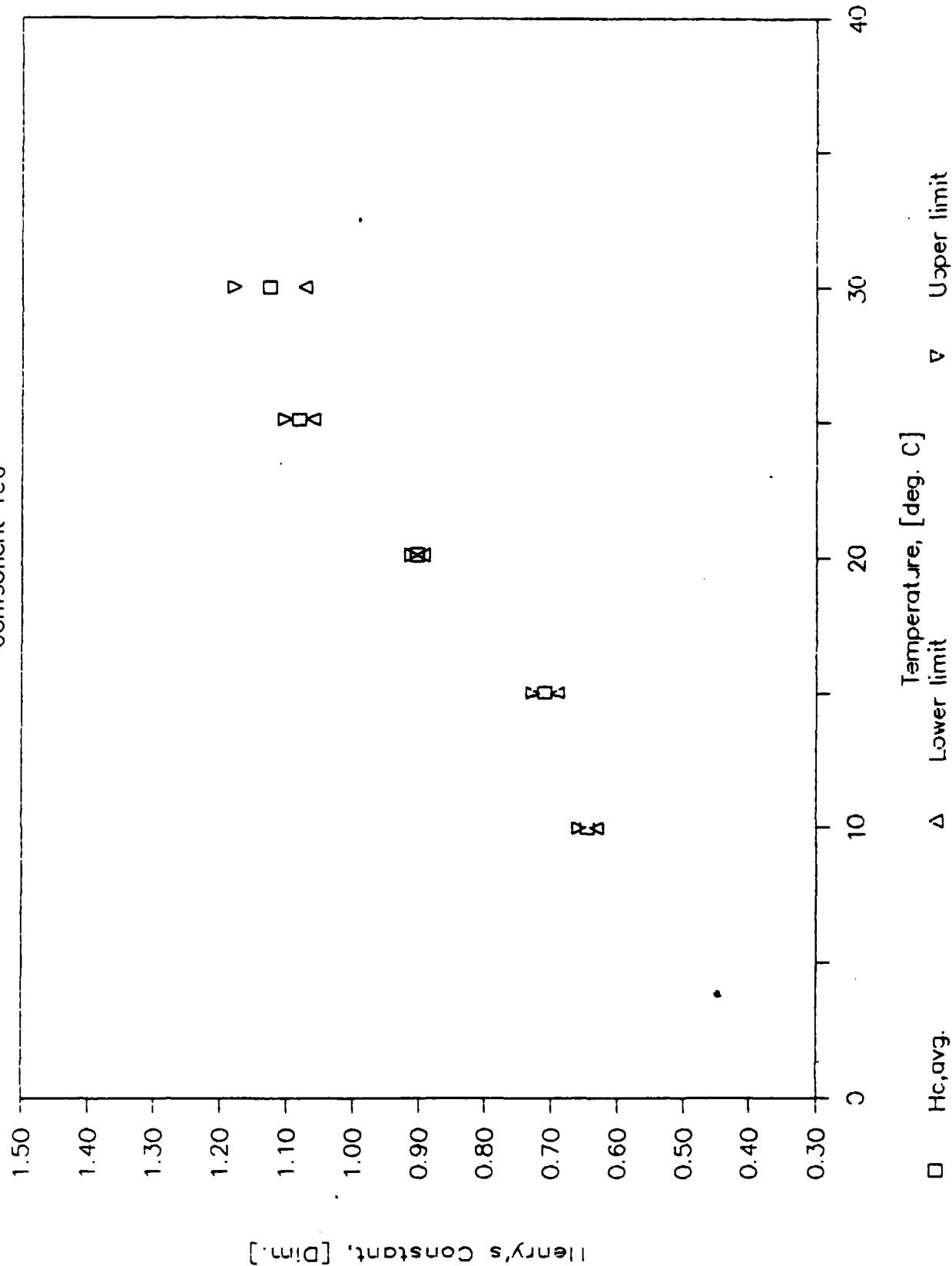
R-SQUARED = 0.9700

TEMPERATURE REGRESSION PLOT



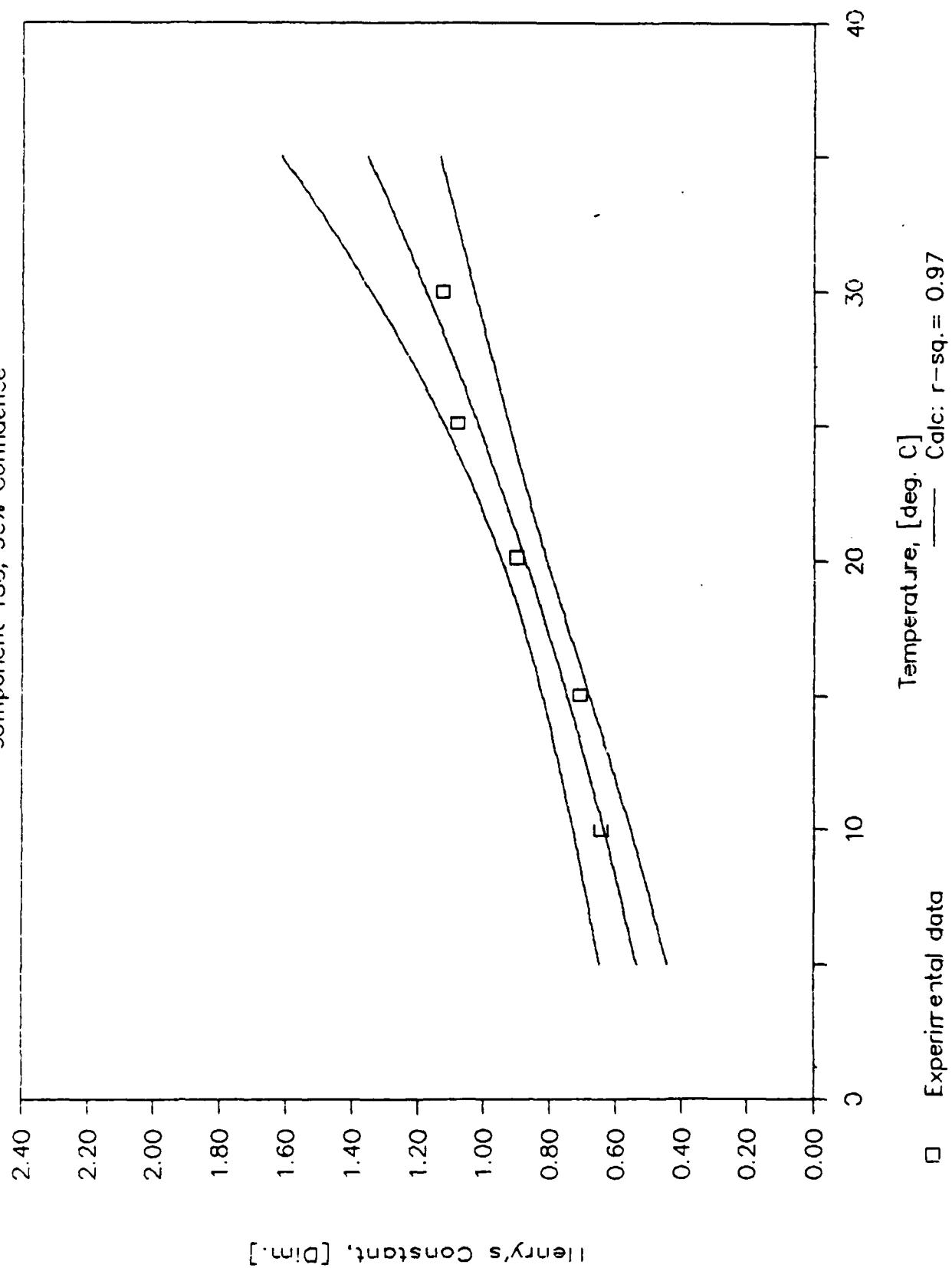
95% CONFIDENCE TEST
Component 130

248



REGRESSION CONFIDENCE TEST

Component 130, 95% Confidence



06-Nov-86

Results Summary for Component 31

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		2		2		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		8		8		8	
Component ID		31		31		31	
Temperature (C)		18		15		20.2	
Low Vol (ml)		25		25		25	
High Vol (ml)		285		285		285	
System Vol (ml)		250		250		250	
H, avg: atm-m3/mol		0.3268	1.0E-25	0.4053	1.0E-25	0.4562	1.0E-25
H, avg: atm-mol/mol		421.4		531.9		609.6	
H, avg: atm-m3/mol		7.59E-03	1	9.58E-03	1	1.10E-02	1
H, avg: kPa-m3/mol		0.7693		0.9710		1.1128	
COV, r [std/mean]		3.50		1.50		0.99	
COV, both replic.		_____	_____	_____	_____	_____	_____
Observation: (1)		0.3173		0.4000		0.4535	
[atm-m3/mol] (2)		0.3164		0.4122		0.4611	
(3)		0.3371		0.3984		0.4514	
(4)		0.3362		0.4025		0.4590	
Injection: (1)		689720		656590		737300	
[Peak Area] (2)		718730		645670		734900	
(3)		1569000		1255600		1308300	
(4)		1572000		1246500		1292900	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		3		3	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		8		8	
Component ID		31		31	
Temperature (C)		25		30	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.4951 1.0E-25		0.5746 1.0E-25	
H, avg: atm-mol/mol		672.3		793.4	
H, avg: atm-m3/mol		1.21E-02	1	1.43E-02	1
H, avg: kPa-m3/mol		1.2274		1.4484	
COV, r [std/mean]		1.46		0.59	
COV, both replic.		_____		_____	
Observation: (1)		0.4925		0.5712	
[atm-m3/m3] (2)		0.4867		0.5722	
(3)		0.5036		0.5770	
(4)		0.4976		0.5788	
Injection: (1)		1857500		780960	
[Peak Area] (2)		1874500		786730	
(3)		1768700		1173600	
(4)		1784000		1172100	

Temperature Regression Parameters:

OF POINTS = 5

SLOPE = -2.6E+03

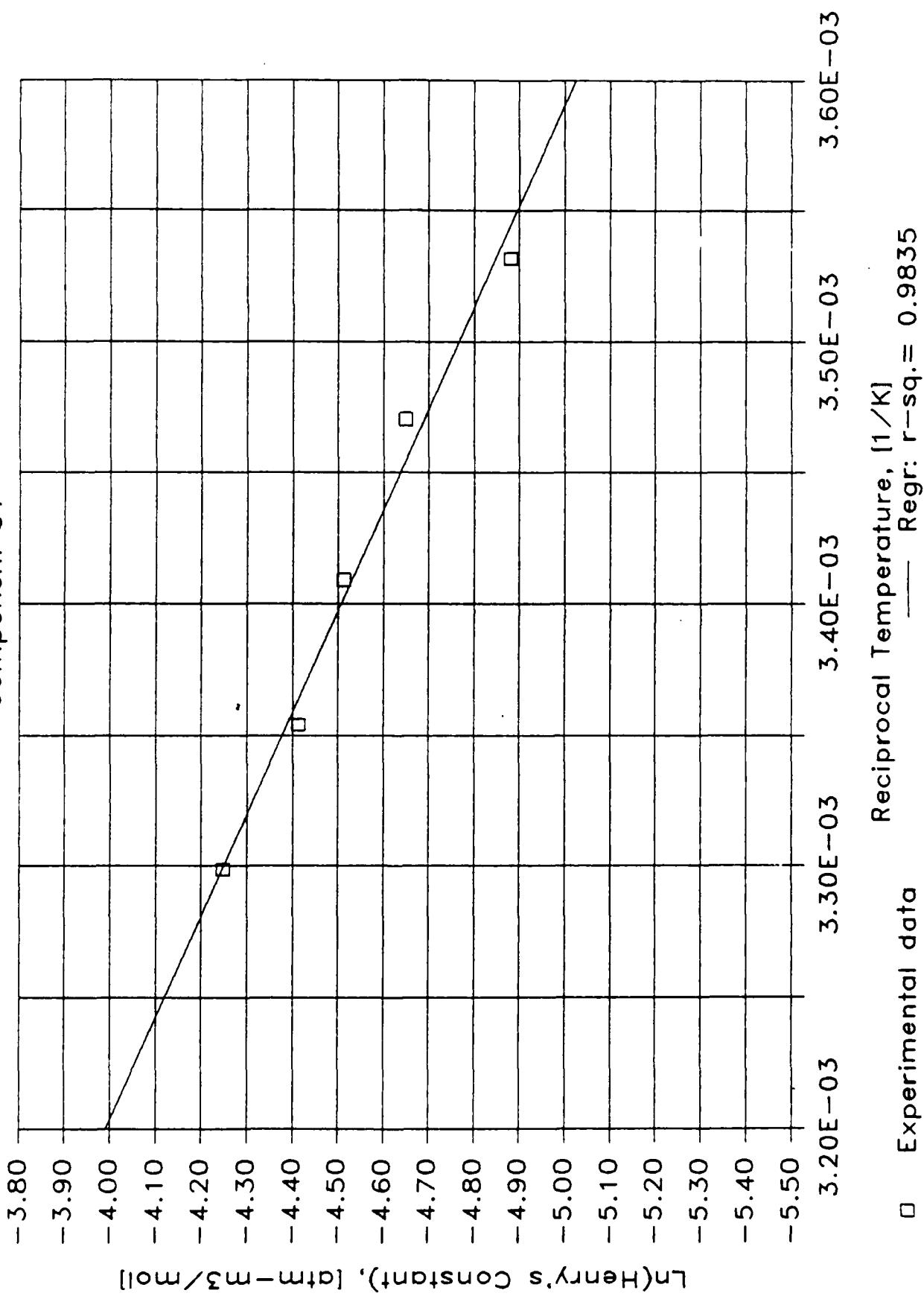
Y-INTERCEPT = 4.3E+00

R-SQUARED = 0.9835

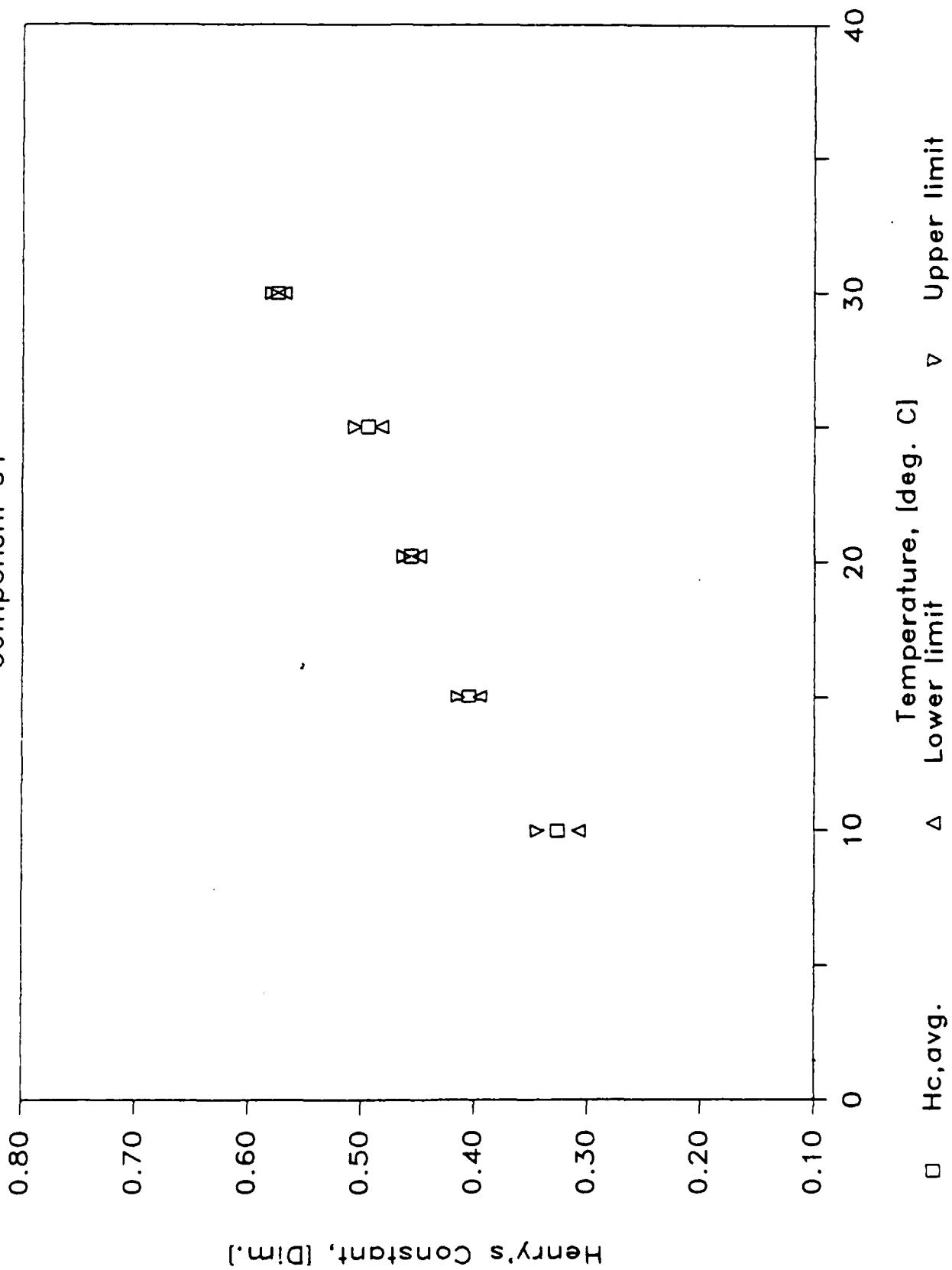
TEMPERATURE REGRESSION PLOT

Component 31

252

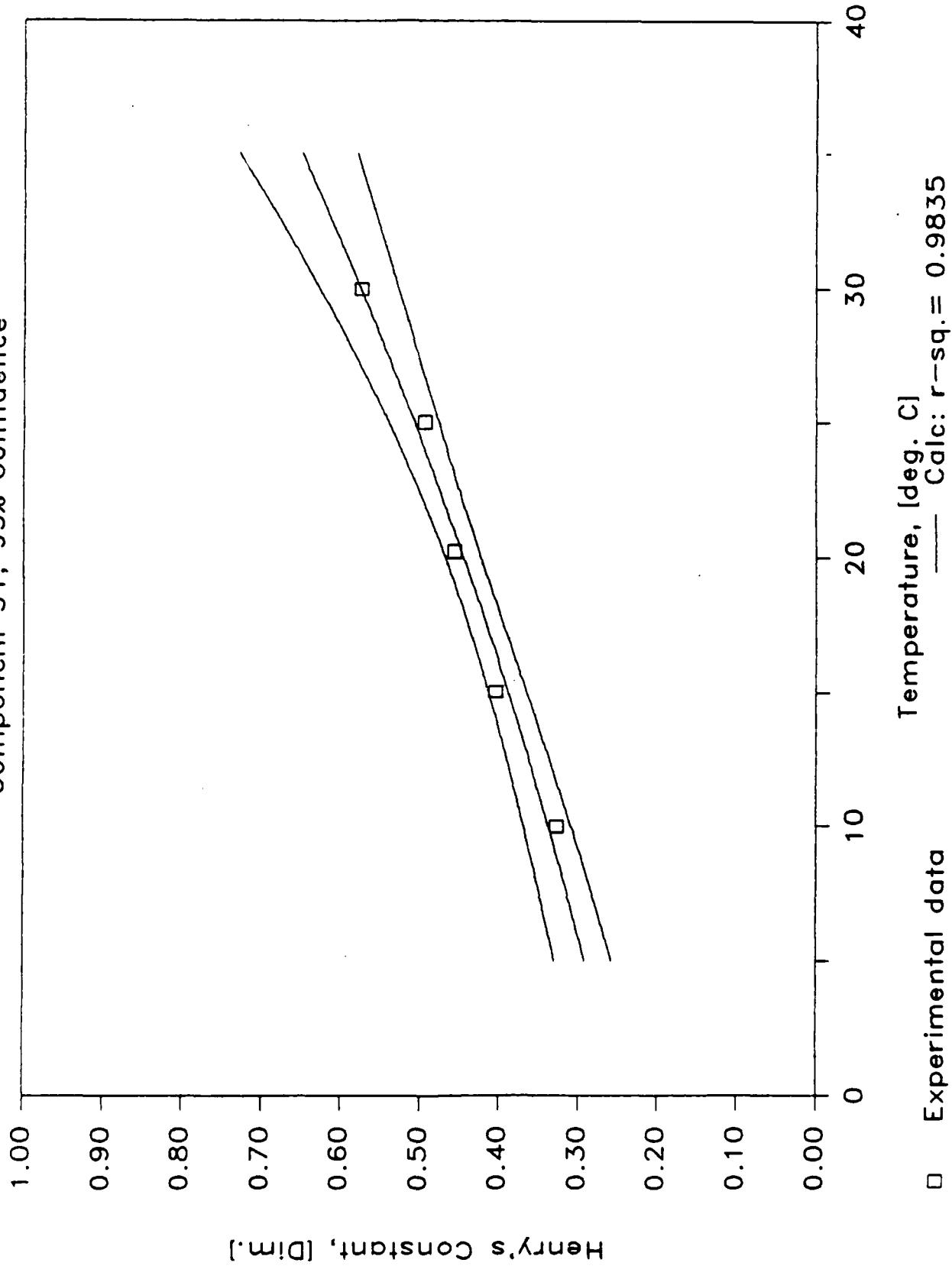


95% CONFIDENCE TEST
Component 31



REGRESSION CONFIDENCE TEST

Component 31, 95% Confidence



86-Nov-86

Results Summary for Component 32

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		6		6		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		8		8		8	
Component ID		32		32		32	
Temperature (C)		10		15		20.2	
Low Vol (ml)		24		24		24	
High Vol (ml)		204		204		204	
System Vol (ml)		250		250		250	
H _c avg: atm-m ³ /m ³		0.2552	1.0E-25	0.2371	1.0E-25	0.2456	1.0E-25
H _c avg: atm-mol/mol		329.1		311.2		328.2	
H _c avg: atm-m ³ /mol		5.93E-03	1	5.61E-03	1	5.91E-03	1
H _c avg: kPa-m ³ /mol		0.6007		0.5681		0.5991	
COV, r [std/mean]		5.28		7.23		21.26	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.2396		0.2363		0.2008	
[atm-m ³ /m ³] (2)		0.2500		0.2584		0.2903	
(3)		0.2600		0.2165		0.2008	
(4)		0.2710		0.2372		0.2914	
Injection: (1)		15413		17300		20556	
[Peak Area] (2)		16250		16442		20687	
(3)		42400		48241		63337	
(4)		41259		45532		49862	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		7		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		8		8	
Component ID		32		32	
Temperature (C)		25		39	
Low Vol (ml)		24		24	
High Vol (ml)		284		284	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.3411 1.0E-25		0.4151 1.0E-25	
H, avg: atm-mol/mol		463.3		573.1	
H, avg: atm-m3/mol		8.35E-03	1	1.03E-02	1
H, avg: kPa-m3/mol		0.8457		1.0463	
COV, r [std/mean]		1.48		4.66	
COV, both replic.		_____		_____	
Observation: (1)		0.3438		0.3936	
(atm-m3/m3) (2)		0.3353		0.4053	
(3)		0.3470		0.4244	
(4)		0.3392		0.4370	
Injection: (1)		26673		32169	
[Peak Area] (2)		26888		33937	
(3)		57740		63256	
(4)		58662		61954	

Temperature Regression Parameters:

OF POINTS = 5

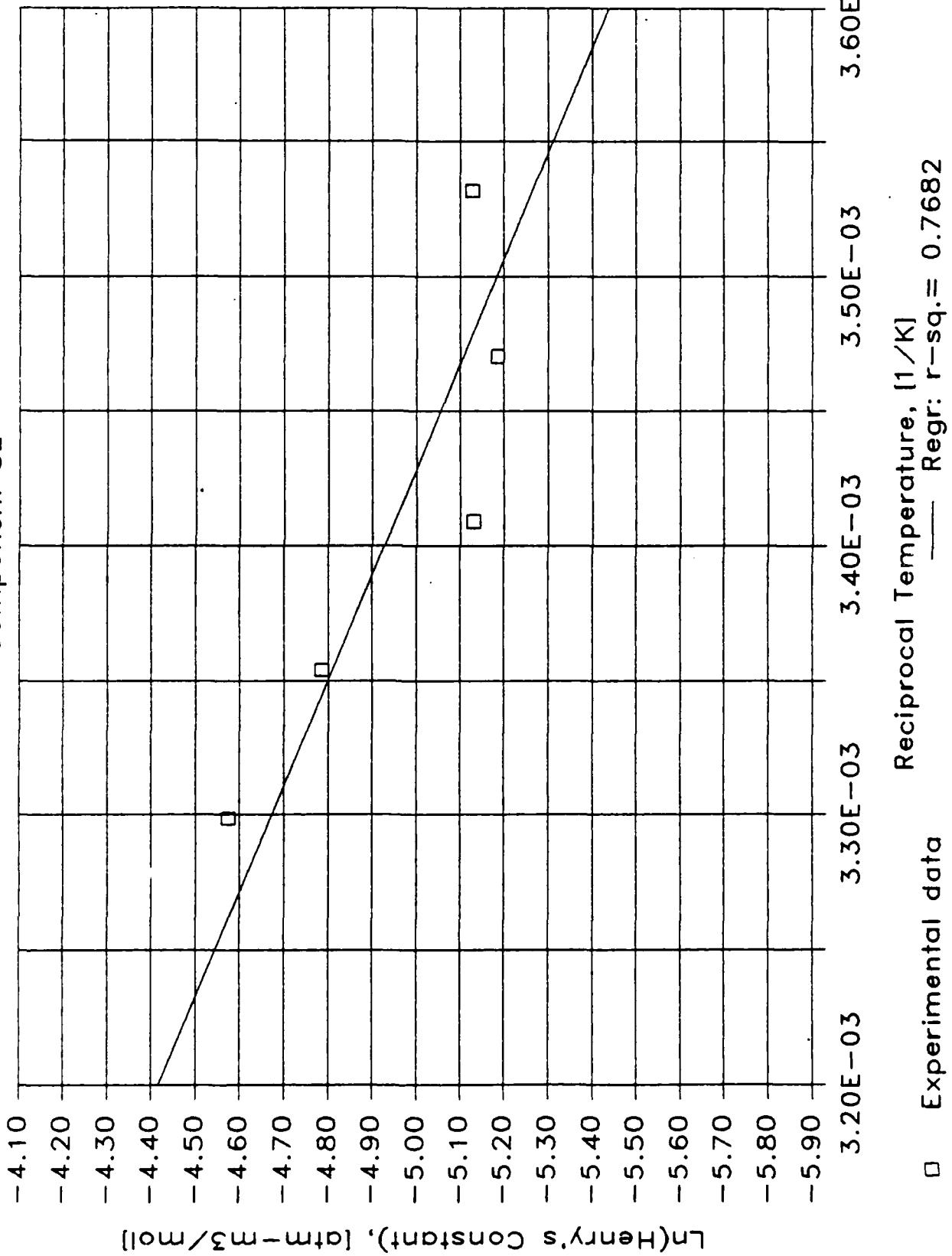
SLOPE = -2.6E+03

Y-INTERCEPT = 3.7E+00

R-SQUARED = 0.7682

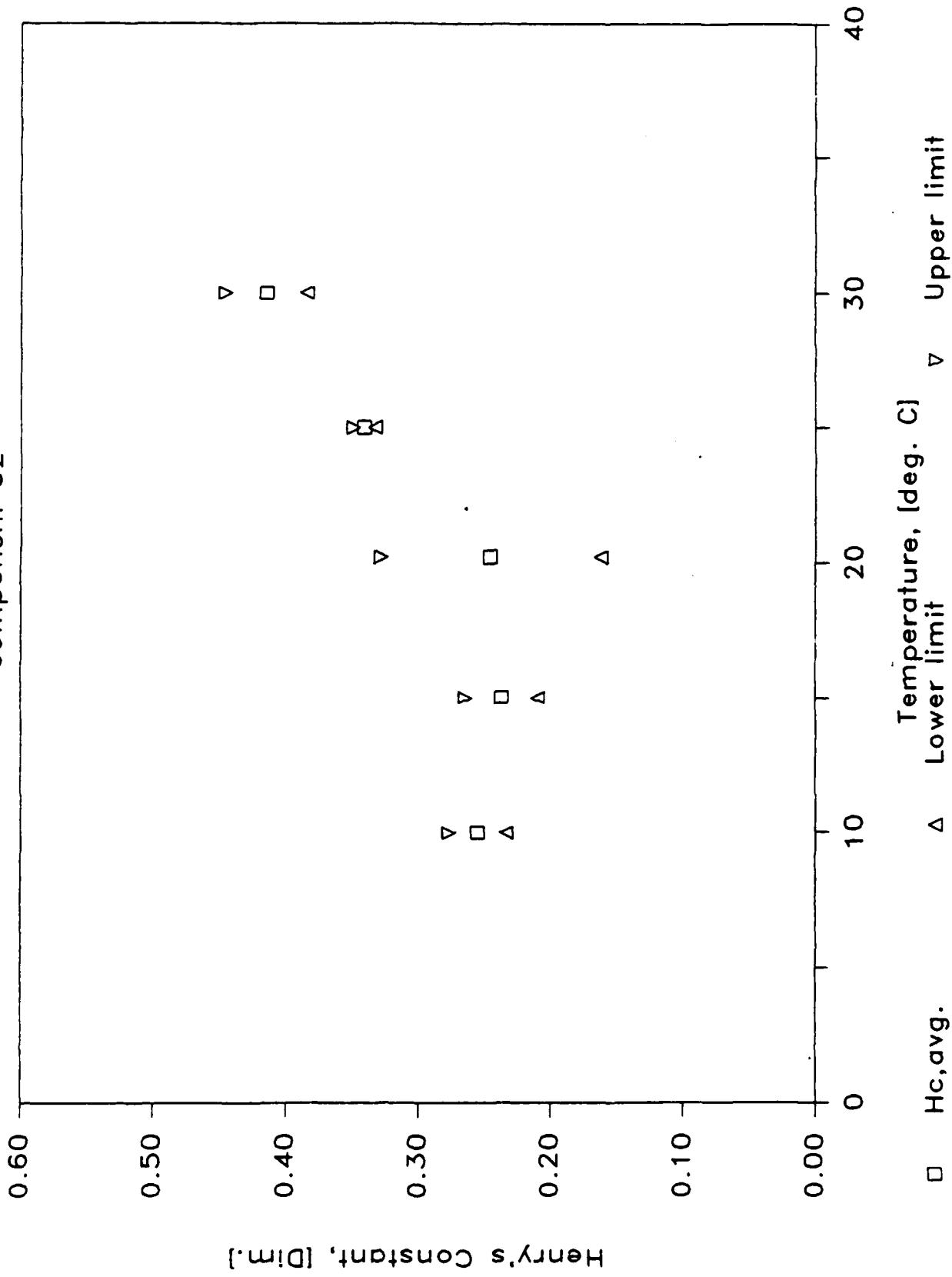
TEMPERATURE REGRESSION PLOT

Component 32



95% CONFIDENCE TEST
Component 32

258

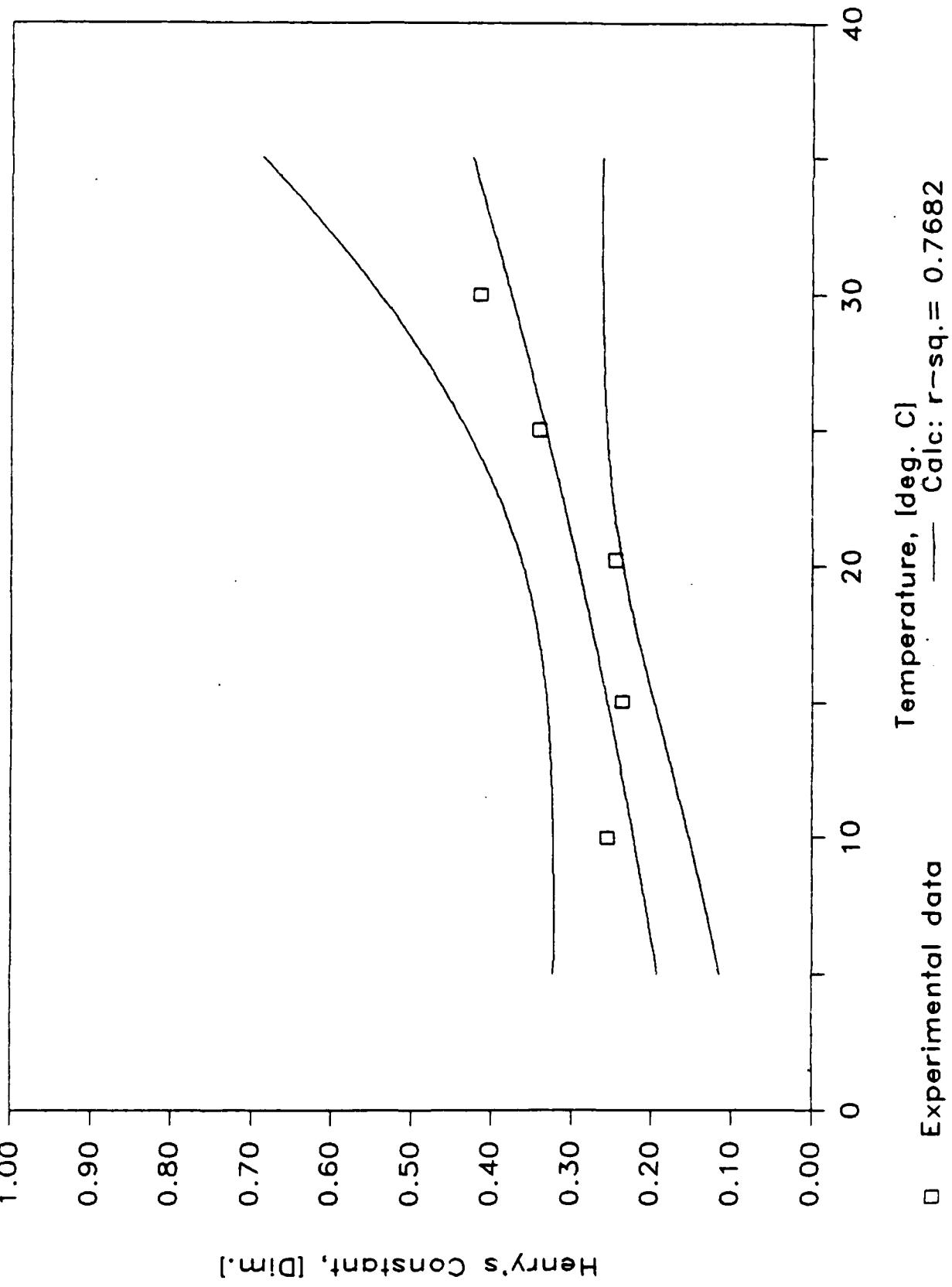


REGRESSION CONFIDENCE TEST

Component 32, 95% Confidence

259

Henry's Constant, [Dim.]



RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	15		15		15	
Component ID	132		132		132	
Temperature (C)	10		15.2		19.9	
Low Vol (ml)	24		24		24	
High Vol (ml)	204		204		204	
System Vol (ml)	250		250		250	
H _v avg: atm-m3/m3	0.0921	1.0E-25	0.3077	1.0E-25	0.2412	1.0E-25
H _v avg: atm-mol/mol	118.7		404.1		321.9	
H _v avg: atm-m3/mol	2.14E-03	1	7.28E-03	1	5.80E-03	1
H _v avg: kPa-m3/mol	0.2168		0.7376		0.5877	
COV, r [std/mmHg]	43.00		6.63		4.61	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.1318		0.3003		0.2488	
[atm-m3/m3] (2)	0.1201		0.3402		0.2299	
(3)	0.0622		0.2764		0.2525	
(4)	0.0541		0.3137		0.2335	
Injection: (1)	8663		13347		16237	
[Peak Area] (2)	6225		12625		16395	
(3)	33831		31643		43606	
(4)	35484		29060		45863	

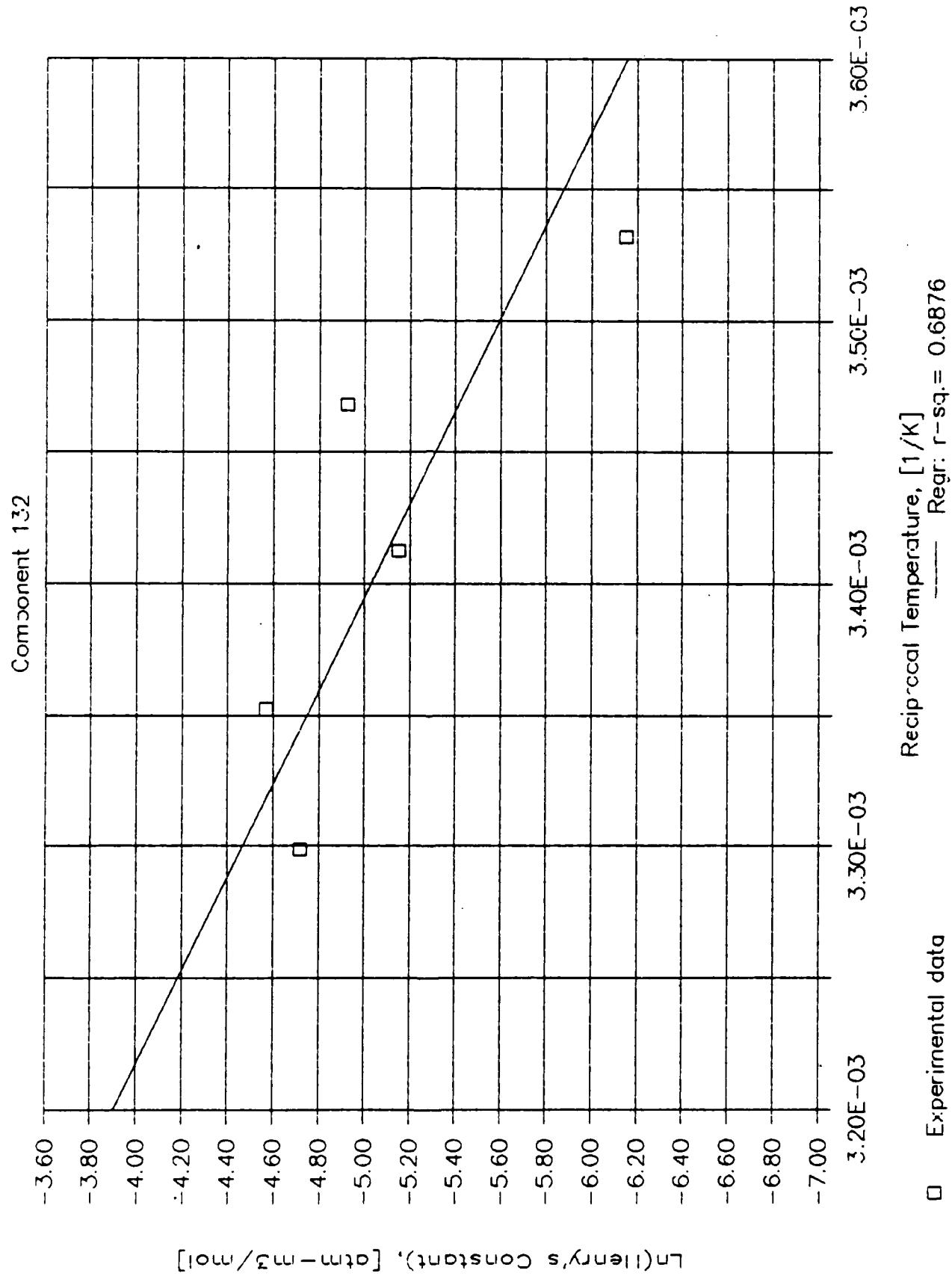
RUN Number -->	Temperature 4		Temperature 5	
	79	No. 1 No. 2	65	No. 1 No. 2
REPLICATE -->				
Group No.		15		15
Component ID		132		132
Temperature (C)		25.15		30
Low Vol (ml)		24		24
High Vol (ml)		204		204
System Vol (ml)		250		250
H, avg: atm-m3/m3		0.4235 1.0E-25		0.3595 1.0E-25
H, avg: atm-mol/mol		575.5		496.5
H, avg: atm-m3/mol		1.04E-02	1	8.94E-03 1
H, avg: kPa-m3/mol		1.0505		0.9063
COV, r [std/mean]		14.83		21.65
COV, both replic.		_____		_____
Observation: (1)		0.4888		0.3850
[atm-m3/m3] (2)		0.4649		0.2735
(3)		0.3798		0.4542
(4)		0.3607		0.3255
Injection: (1)		22732		25816
[Peak Area] (2)		18988		29033
(3)		38287		51556
(4)		39698		65164

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

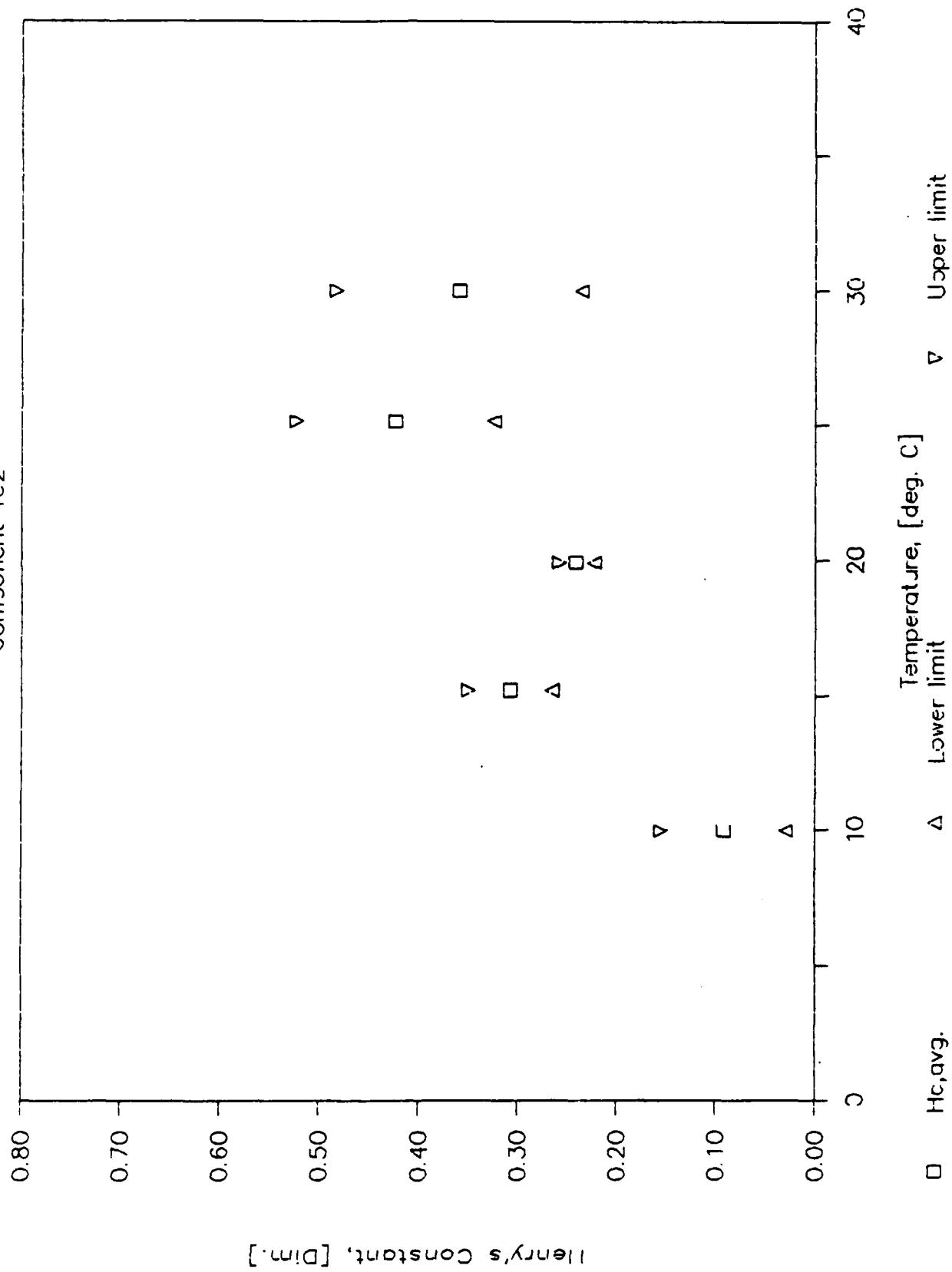
OF POINTS = 5
 SLOPE = -5.6E+03
 Y-INTERCEPT = 1.4E+01
 R-SQUARED = 0.6876

TEMPERATURE REGRESSION PLOT



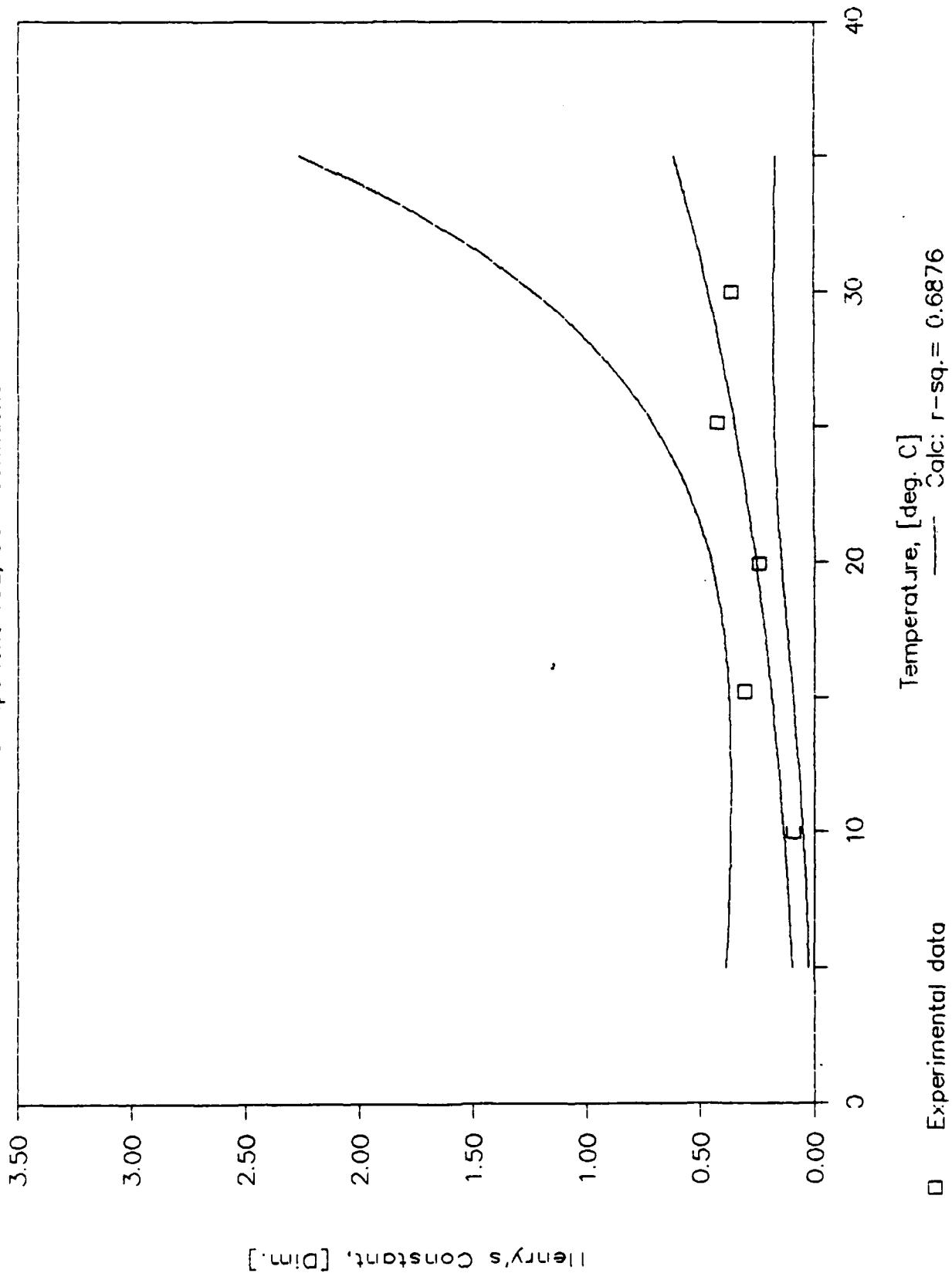
95% CONFIDENCE TEST

Component 132



REGRESSION CONFIDENCE TEST

Component 132, 95% Confidence



06-Nov-86

Results Summary for Component 33

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE →						
Group No.	8		8		8	
Component ID	33		33		33	
Temperature (C)	10		15		20.2	
Low Vol (ml)	22		22		22	
High Vol (ml)	202		202		202	
System Vol (ml)	250		250		250	
H, avg: atm-m3/m3	0.6386	1.0E-25	0.8883	1.0E-25	0.9653	1.0E-25
H, avg: atm-mol/mol	823.6		1060.9		1289.8	
H, avg: atm-m3/mol	1.48E-02	1	1.91E-02	1	2.32E-02	1
H, avg: kPa-m3/mol	1.5035		1.9366		2.3545	
COV, r [std/mean]	1.28		3.98		3.41	
COV, both replic.	—		—		—	
Observation: (1)	0.6336		0.8833		0.9497	
[atm-m3/m3] (2)	0.6300		0.8471		0.9283	
(3)	0.6473		0.7704		1.0029	
(4)	0.6435		0.8124		0.9802	
Injection: (1)	376200		393720		454690	
[Peak Area] (2)	382240		381840		472930	
(3)	525350		461660		471940	
(4)	527600		444080		479800	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		11		10	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		8		8	
Component ID		33		33	
Temperature (C)		25		30	
Low Vol (ml)		22		22	
High Vol (ml)		202		202	
System Vol (ml)		250		250	
H _c avg: atm-m ³ /m ³		1.2036	1.0E-25	1.5210	1.0E-25
H _c avg: atm-mol/mol		1634.5		2100.2	
H _c avg: atm-m ³ /mol		2.94E-02	1	3.78E-02	1
H _c avg: kPa-m ³ /mol		2.9837		3.8338	
COV, r [std/mean]		2.25		5.93	
COV, both replic.		_____		_____	
Observation: (1)		1.2332		1.4176	
[atm-m ³ /m ³] (2)		1.1881		1.5524	
(3)		1.2188		1.4856	
(4)		1.1743		1.6283	
Injection: (1)		637490		485580	
[Peak Area] (2)		632260		501320	
(3)		549240		379840	
(4)		563790		357150	

Temperature Regression Parameters:

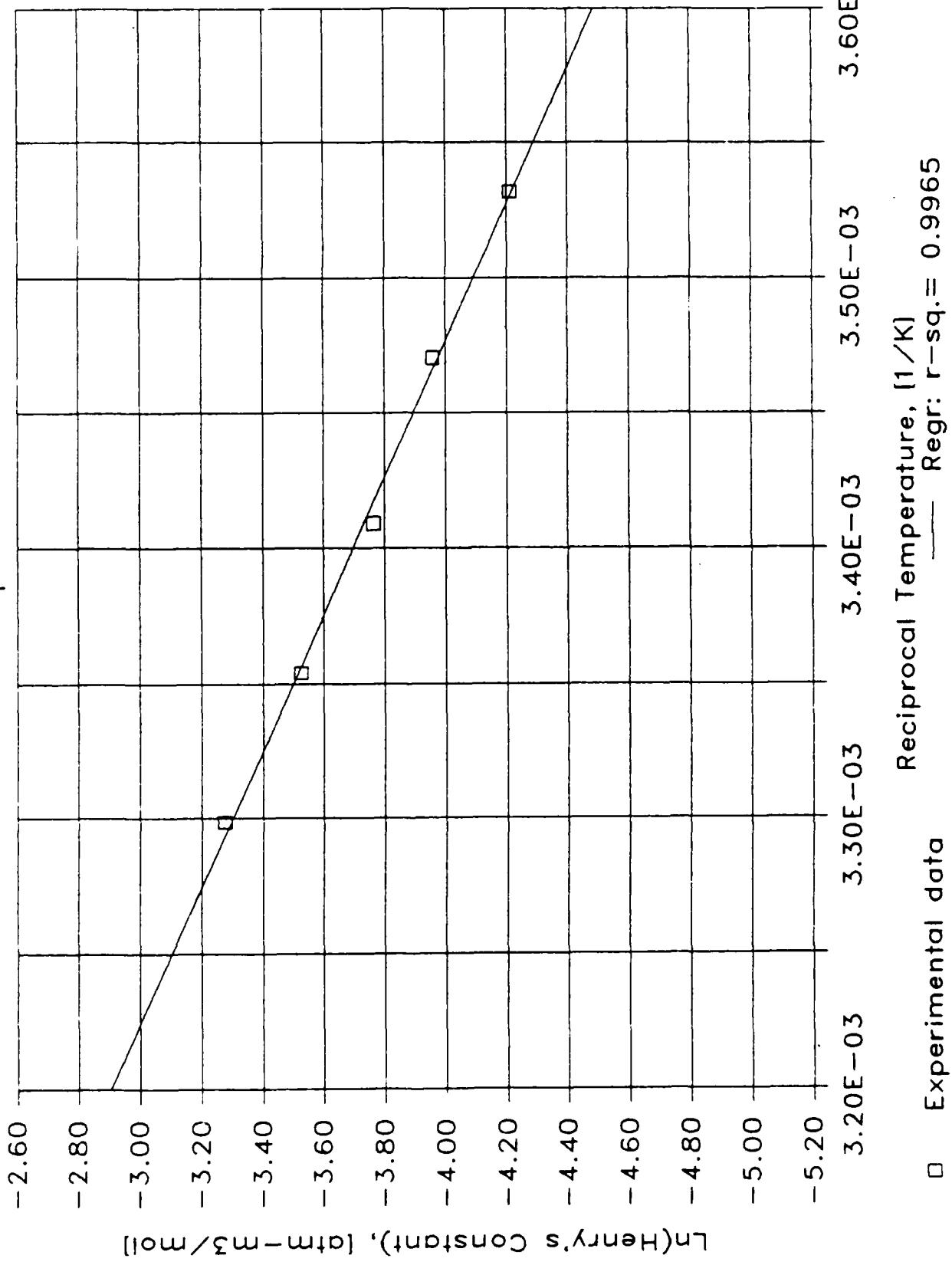
OF POINTS = 5

SLOPE = -4.0E+03

Y-INTERCEPT = 9.7E+00

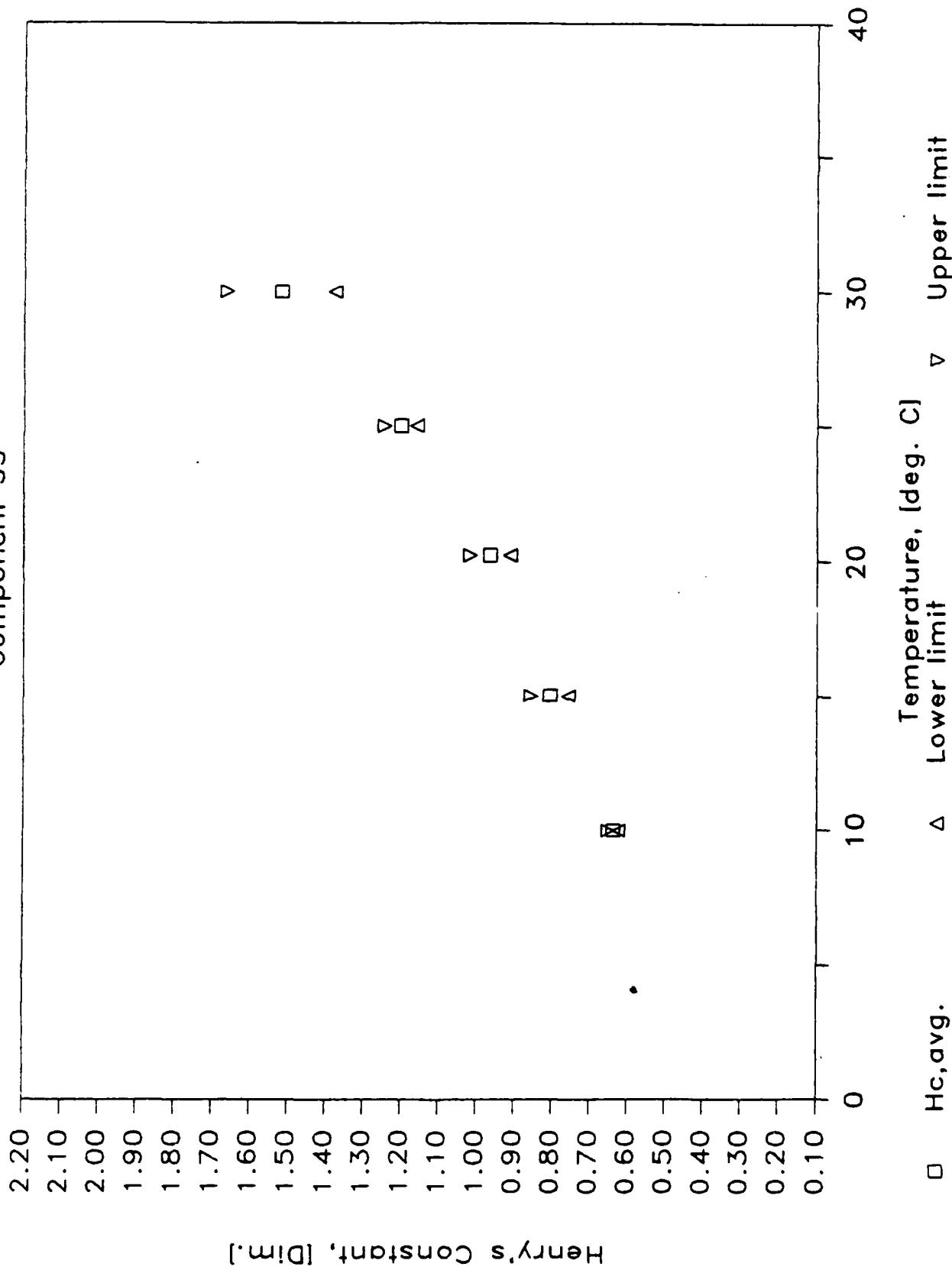
R-SQUARED = 0.9965

TEMPERATURE REGRESSION PLOT
Component 33



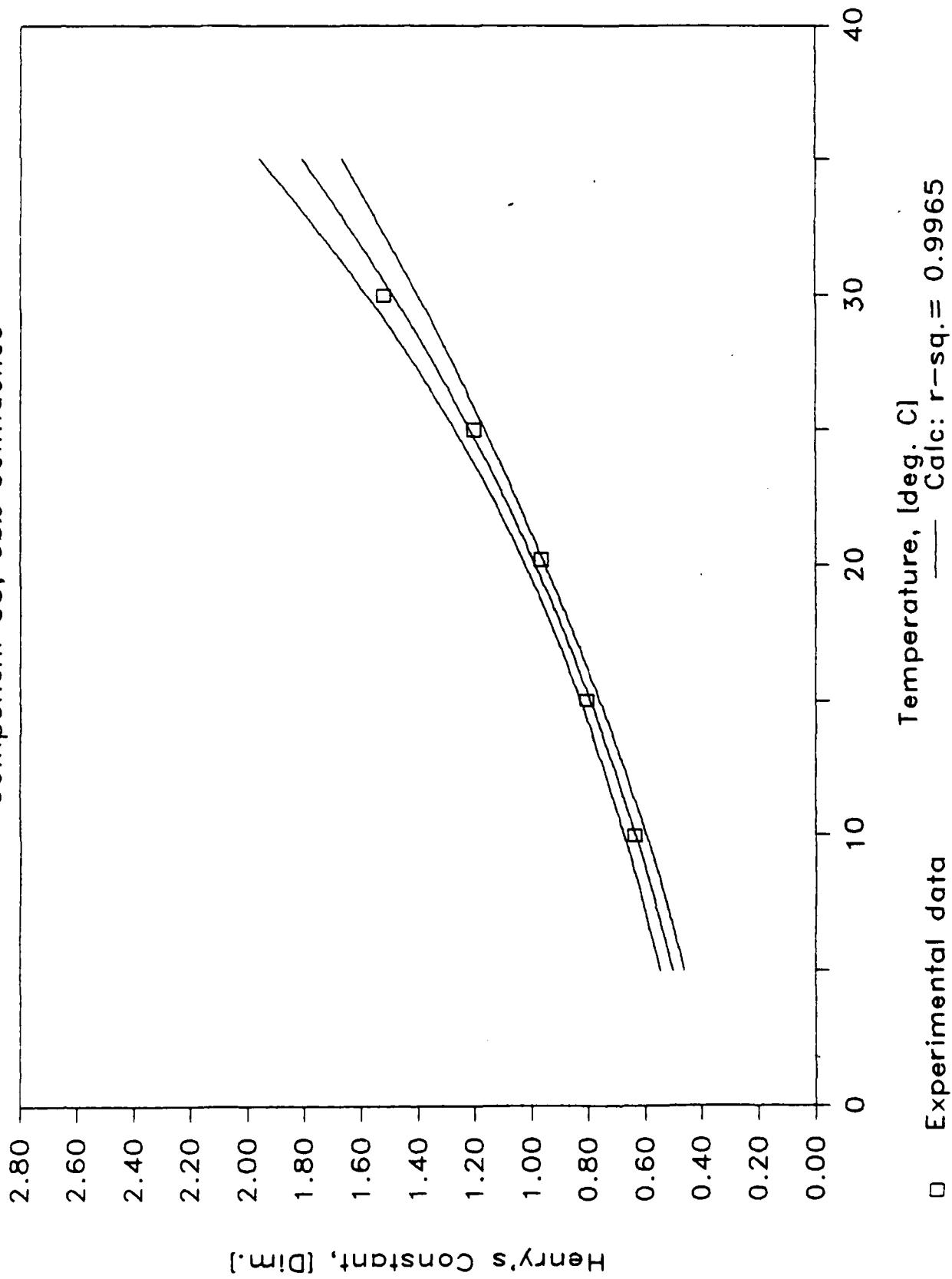
95% CONFIDENCE TEST
Component 33

268



REGRESSION CONFIDENCE TEST

Component 33, 95% Confidence



06-Nov-86

Results Summary for Component 34

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		6		6		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		4		4		4	
Component ID		34		34		34	
Temperature (C)		18		14.9		20.1	
Low Vol (ml)		30		30		30	
High Vol (ml)		210		210		210	
System Vol (ml)		250		250		250	
H, avg: atm=m3/m3		0.1733	1.0E-25	0.1945	1.0E-25	0.2374	1.0E-25
H, avg: atm=mol/mol		223.5		255.1		317.1	
H, avg: atm=m3/mol		4.03E-03	1	4.60E-03	1	5.71E-03	1
H, avg: kPa=m3/mol		0.4088		0.4657		0.5788	
COV, r [std/mean]		4.52		1.89		4.81	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.1829		0.1988		0.2284	
[atm=m3/m3] (2)		0.1745		0.1934		0.2482	
(3)		0.1720		0.1955		0.2266	
(4)		0.1639		0.1901		0.2463	
Injection: (1)		113840		174540		222800	
[Peak Area] (2)		110170		172910		221780	
(3)		352230		515850		608350	
(4)		361220		523870		579170	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		7		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		4		4	
Component ID		34		34	
Temperature (C)		25		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.2752	1.0E-25	0.3870	1.0E-25
H, avg: atm-mol/mol		373.7		534.3	
H, avg: atm-m3/mol		6.73E-03	1	9.63E-03	1
H, avg: kPa-m3/mol		0.6822		0.9754	
COV, r [std/mean]		2.70		0.48	
COV, both replic.		_____		_____	
Observation: (1)		0.2672		0.3856	
[atm-m3/mol]	(2)	0.2700		0.3852	
	(3)	0.2795		0.3888	
	(4)	0.2832		0.3884	
Injection:	(1)	232930		396380	
[Peak Area]	(2)	239480		398590	
	(3)	579010		778120	
	(4)	574210		778720	

Temperature Regression Parameters:

OF POINTS = 5

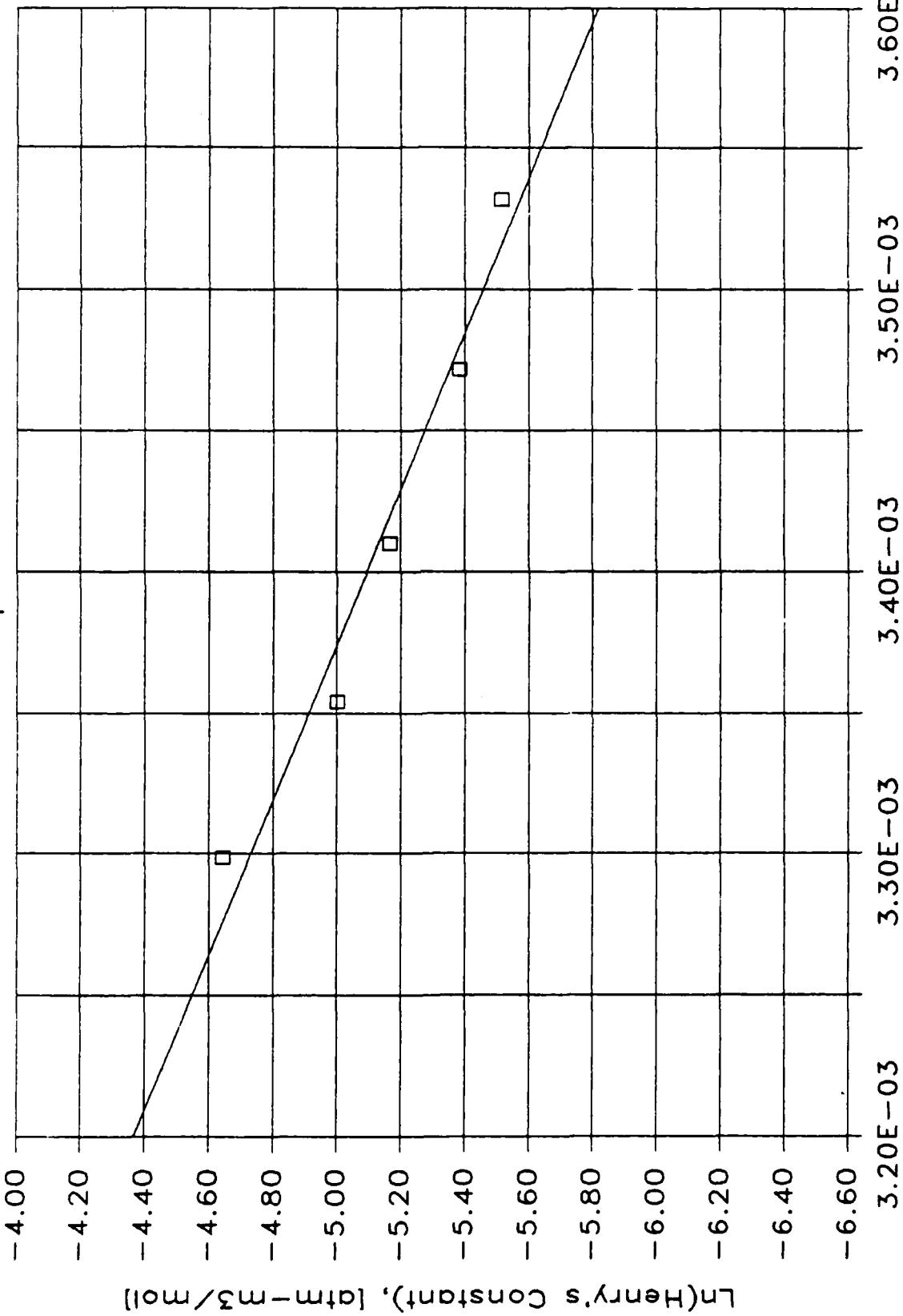
SLOPE = -3.6E+03

Y-INTERCEPT = 7.2E+00

R-SQUARED = 0.9622

TEMPERATURE REGRESSION PLOT

Component 34



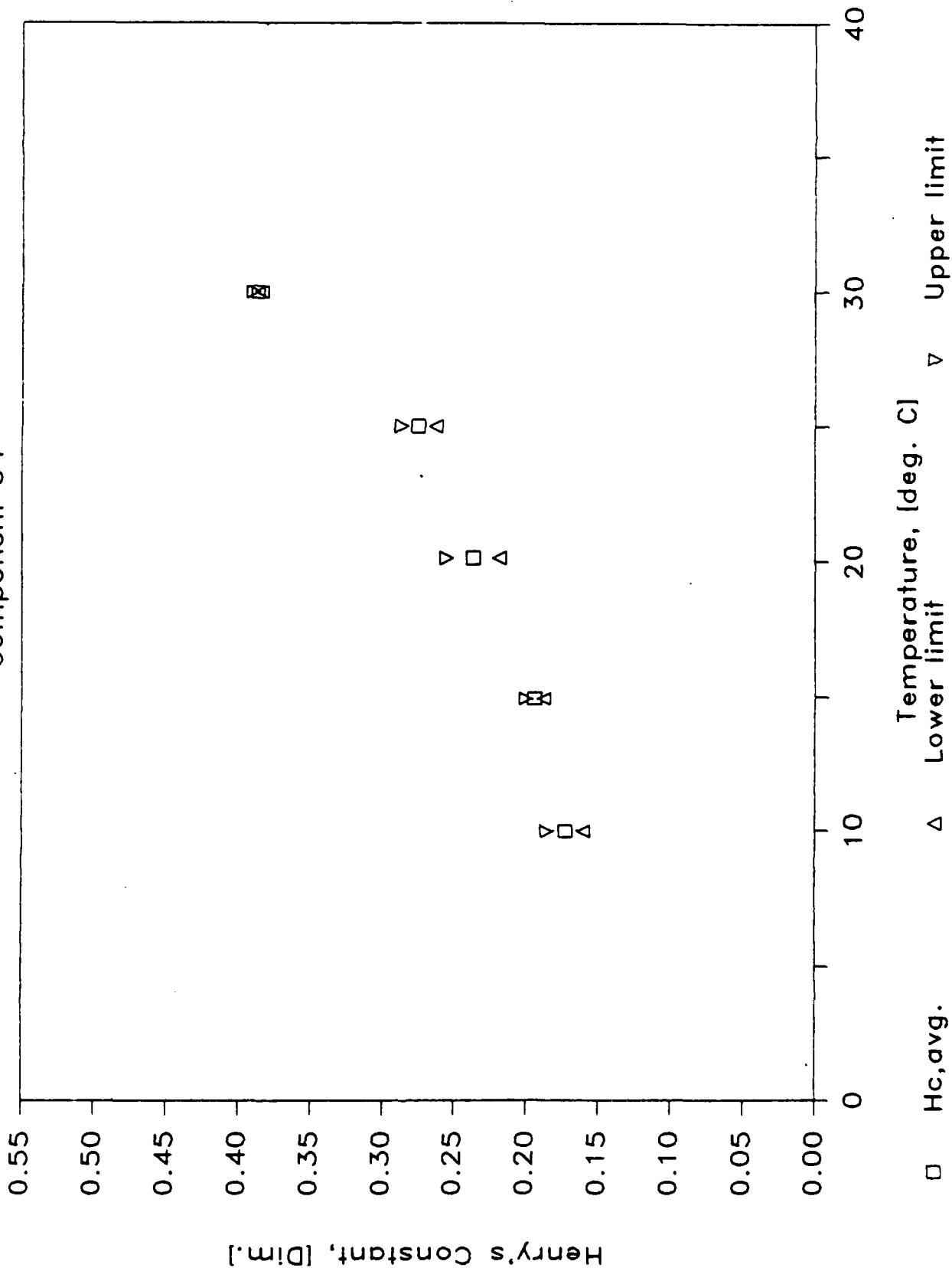
□ Experimental data

Reciprocal Temperature, [1/K]

Regr: r-sq.= 0.9622

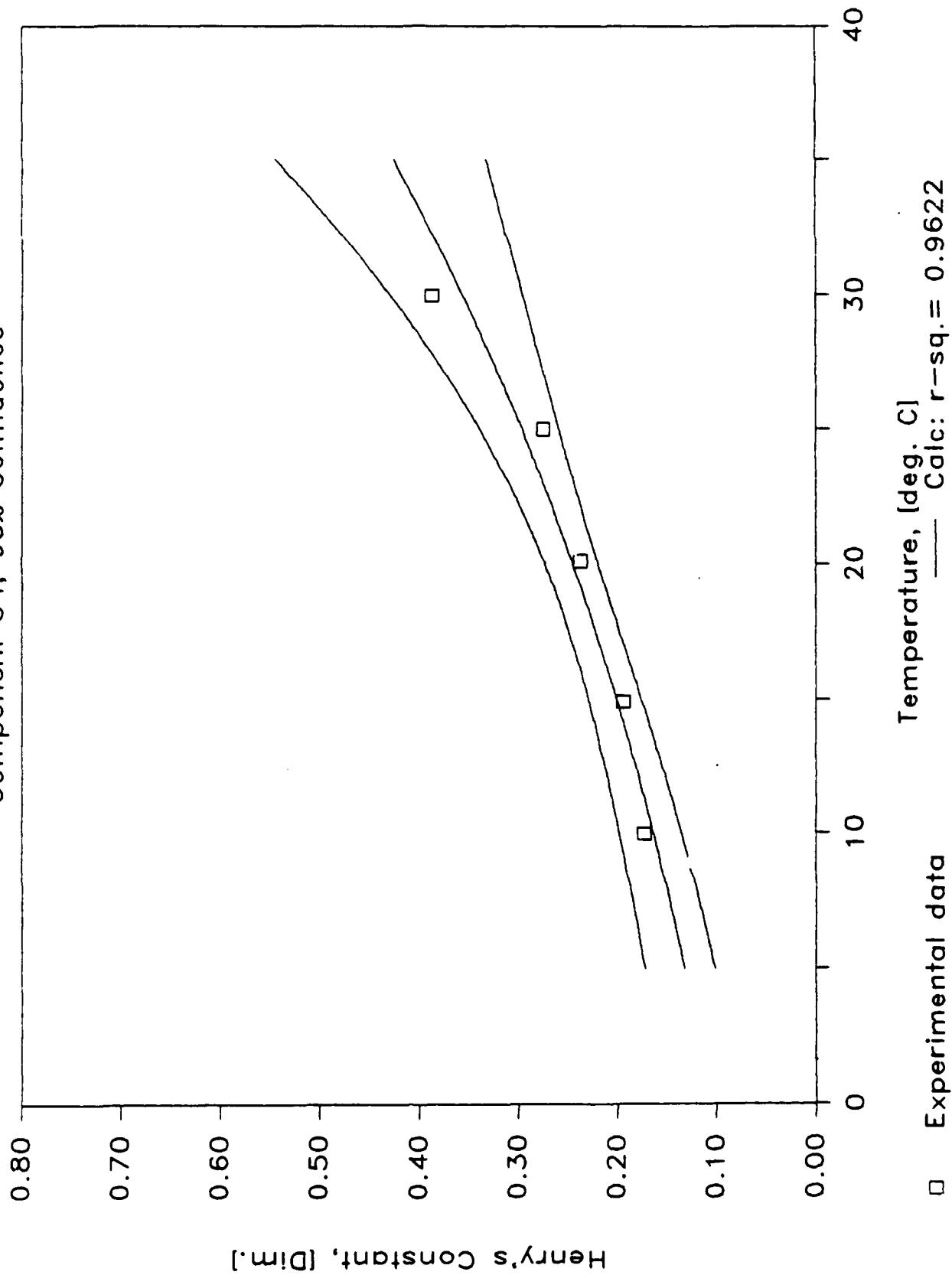
95% CONFIDENCE TEST
Component 34

273



REGRESSION CONFIDENCE TEST
Component 34, 95% Confidence

274



06-Nov-86

Results Summary for Component 36

		Temperature 1		Temperature 2		Temperature 3	
RUN Number	→	7		6		7	
REPLICATE	→	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		9		9		9	
Component ID		36		36		36	
Temperature (C)		18		15		20	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H, avg: atm-m3/m3		0.0533	1.0E-25	0.0269	1.0E-25	0.0194	1.0E-25
H, avg: atm-mol/mol		68.7		35.3		25.9	
H, avg: atm-m3/mol		1.24E-03	1	6.35E-04	1	4.66E-04	1
H, avg: kPa-m3/mol		0.1254		0.0644		0.0472	
COV, r [std/mean]		45.73		7.01		12.23	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.0733		0.0291		0.0194	
[atm-m3/m3] (2)		0.0754		0.0276		0.0165	
(3)		0.0314		0.0261		0.0223	
(4)		0.0330		0.0247		0.0194	
Injection: (1)		343770		351950		407640	
[Peak Area] (2)		268070		344730		416580	
(3)		1725500		2302300		2858900	
(4)		1707200		2325100		2921100	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number →		8		7	
REPLICATE →		No. 1	No. 2	No. 1	No. 2
Group No.		9		9	
Component ID		36		36	
Temperature (C)		25		30	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.0215	1.0E-25	0.0315	1.0E-25
H, avg: atm-mol/mol		29.3		43.6	
H, avg: atm-m3/mol		5.27E-04	1	7.85E-04	1
H, avg: kPa-m3/mol		0.0534		0.0795	
COV, r [std/mean]		5.38		16.53	
COV, both replic.		_____		_____	
Observation: (1)		0.0225		0.0370	
[atm-m3/m3] (2)		0.0205		0.0348	
(3)		0.0226		0.0282	
(4)		0.0206		0.0261	
Injection: (1)		493260		884300	
[Peak Area] (2)		493550		833160	
(3)		3380300		5482500	
(4)		3429600		5563600	

Temperature Regression Parameters:

OF POINTS = 5

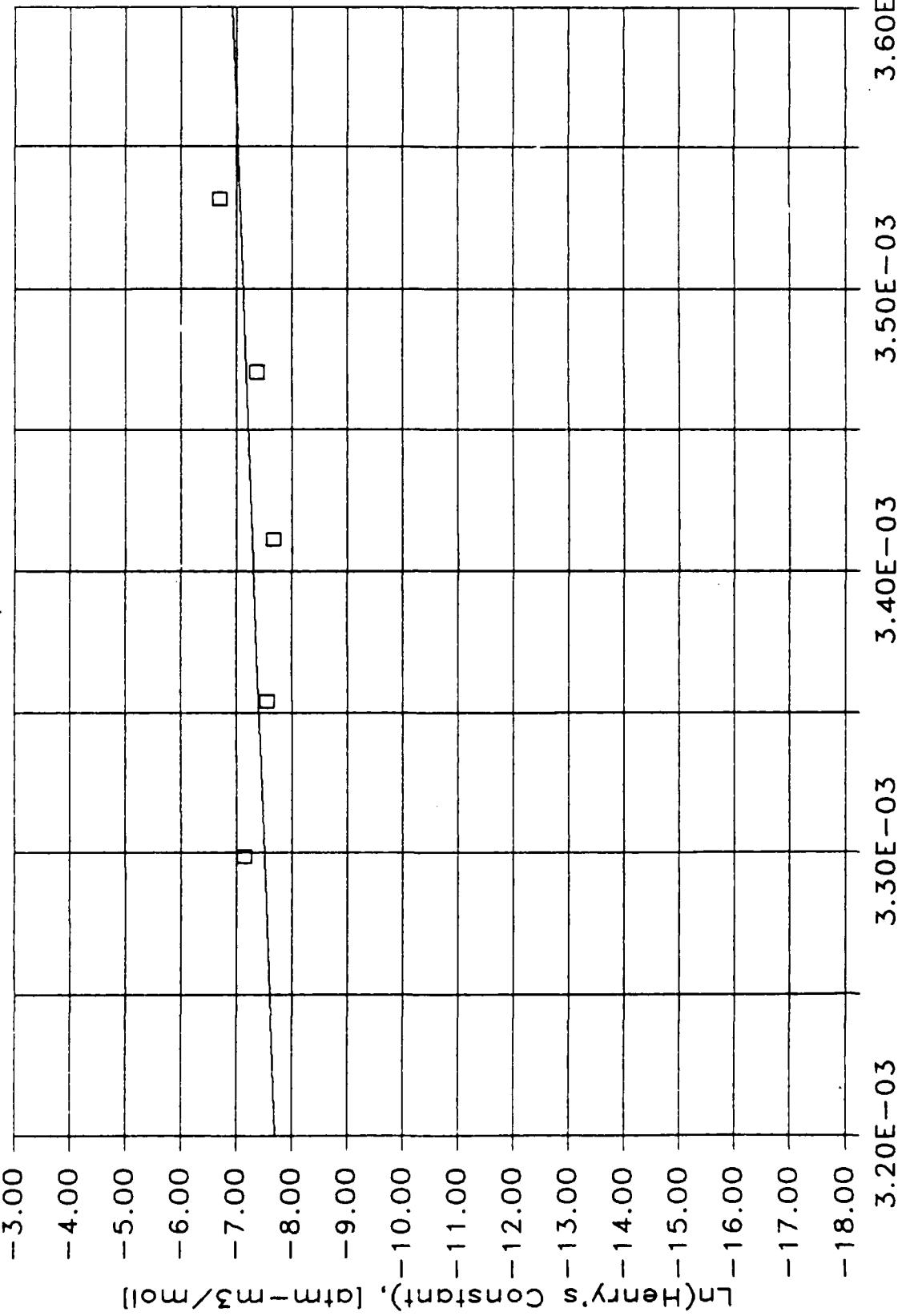
SLOPE = 2.0E+03

Y-INTERCEPT = -1.4E+01

R-SQUARED = 0.2208

TEMPERATURE REGRESSION PLOT

Component 36

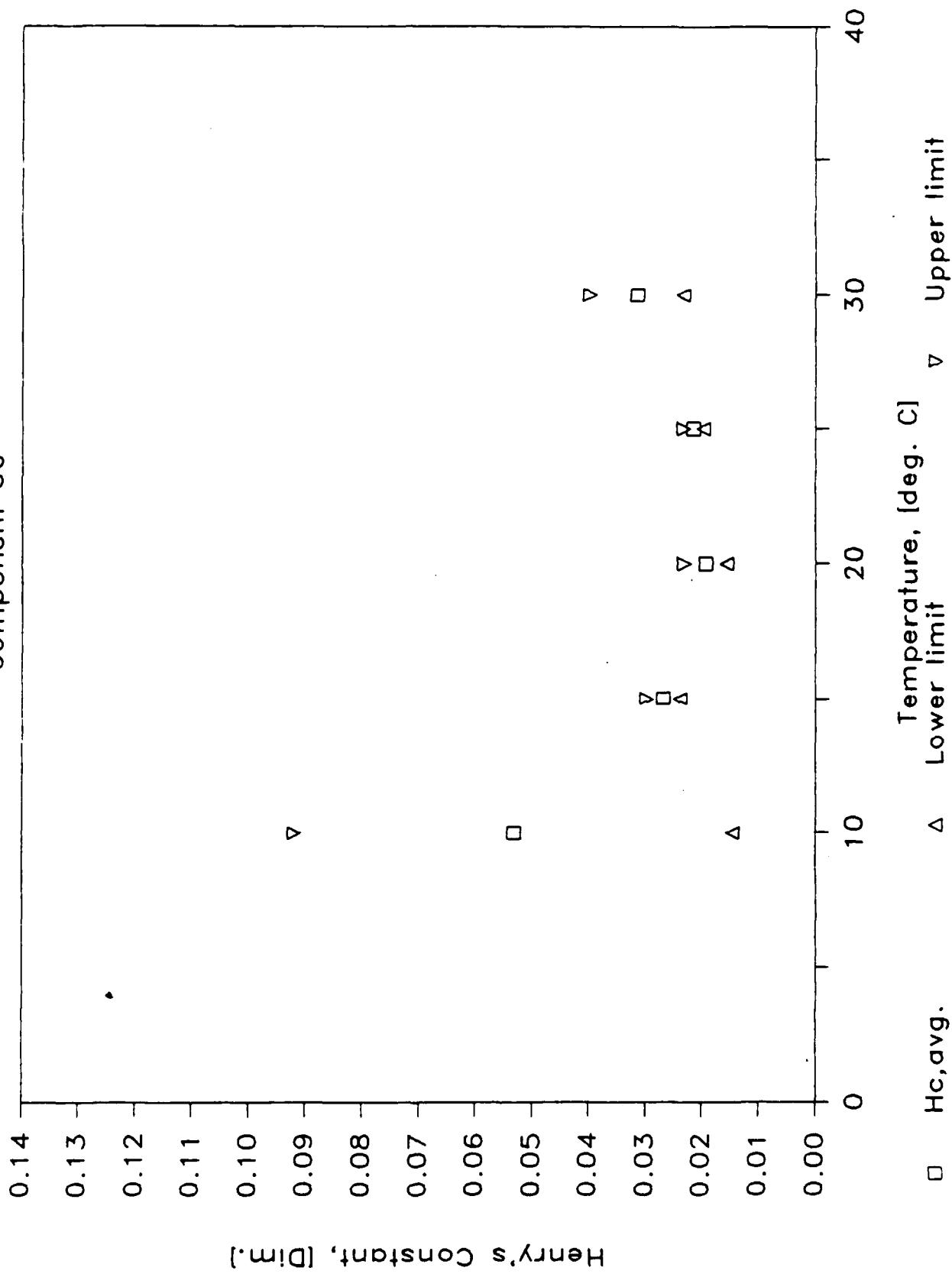


□ Experimental data

Regr: $r_{\text{sq.}} = 0.2208$

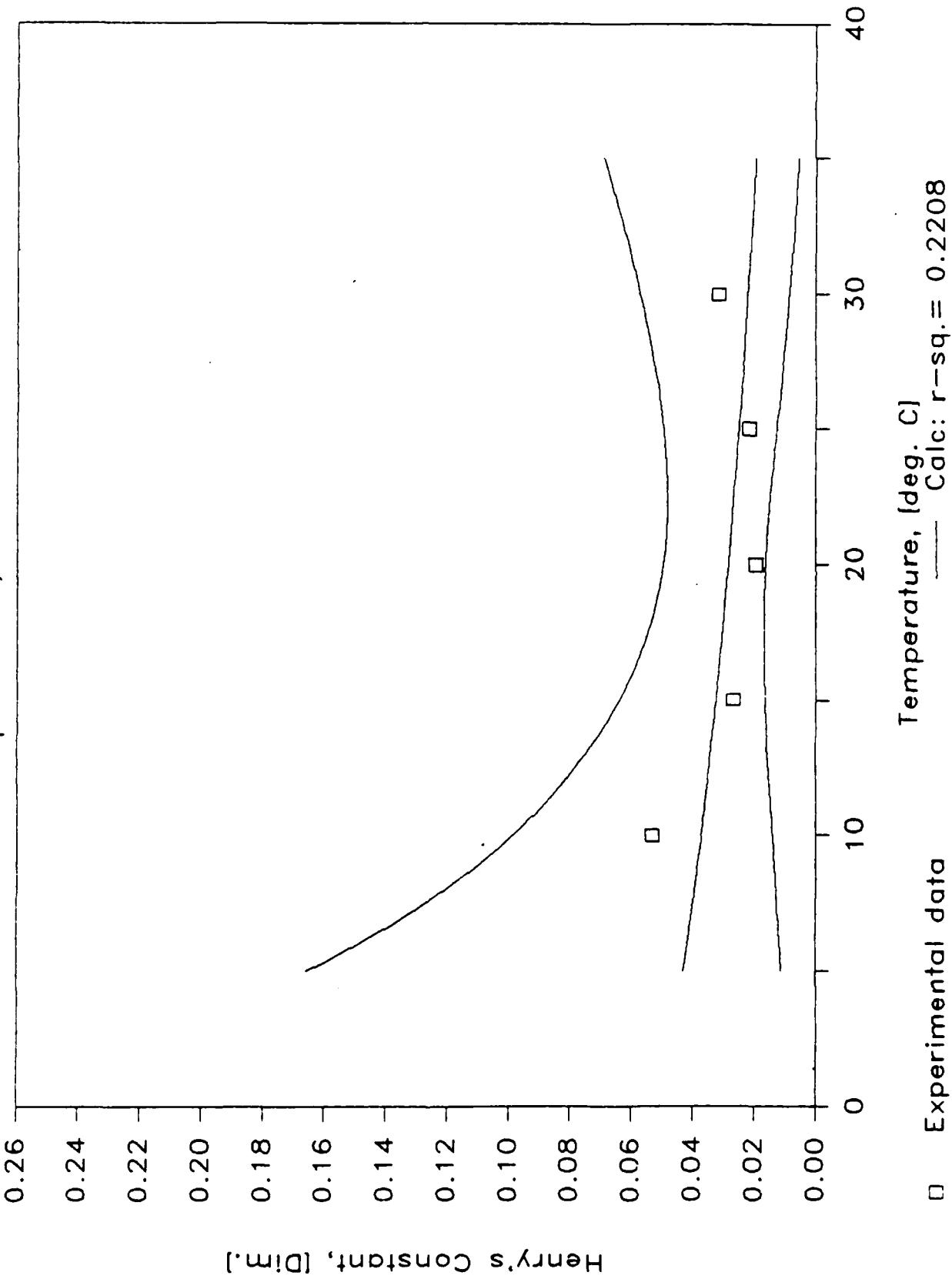
95% CONFIDENCE TEST
Component 36

278



REGRESSION CONFIDENCE TEST

Component 36, 95% Confidence



04-Nov-86

Results Summary for Component 136

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		6		6		5	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		16		16		16	
Component ID		136		136		136	
Temperature (C)		10		15		20.1	
Low Vol (ml)		25		25		25	
High Vol (ml)		205		205		205	
System Vol (ml)		250		250		250	
H _c avg: atm-m3/mol		0.0130	1.0E-25	0.0202	1.0E-25	0.0252	1.0E-25
H _c avg: atm-mol/mol		16.8		26.5		33.6	
H _c avg: atm-m3/mol		3.02E-04	1	4.77E-04	1	6.06E-04	1
H _c avg: kPa-m3/mol		0.0306		0.0483		0.0614	
COV, r [std/mean]		33.19		49.30		52.61	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.0155		0.0237		0.0383	
[atm-m3/mol]	(2)	0.0177		0.0320		0.0349	
	(3)	0.0084		0.0088		0.0152	
	(4)	0.0104		0.0162		0.0124	
Injection:	(1)	92157		78050		111140	
[Peak Area]	(2)	87113		69678		94494	
	(3)	665330		530380		683640	
	(4)	654440		500410		699000	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		7		7	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		16		16	
Component ID		136		136	
Temperature (C)		25.1		30	
Low Vol (ml)		25		25	
High Vol (ml)		205		205	
System Vol (ml)		250		250	
H, avg: atm-m3/m3		0.0267	1.0E-25	0.0320	1.0E-25
H, avg: atm-mol/mol		36.2		44.2	
H, avg: atm-m3/mol		6.53E-04	1	7.96E-04	1
H, avg: kPa-m3/mol		0.0662		0.0806	
COV, r [std/mean]		5.41		7.28	
COV, both replic.					
Observation: (1)		0.0283		0.0342	
[atm-m3/m3] (2)		0.0259		0.0339	
(3)		0.0275		0.0301	
(4)		0.0251		0.0298	
Injection:	(1)	118950		246060	
[Peak Area]	(2)	118320		239450	
(3)		782460		1554800	
(4)		795690		1558000	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

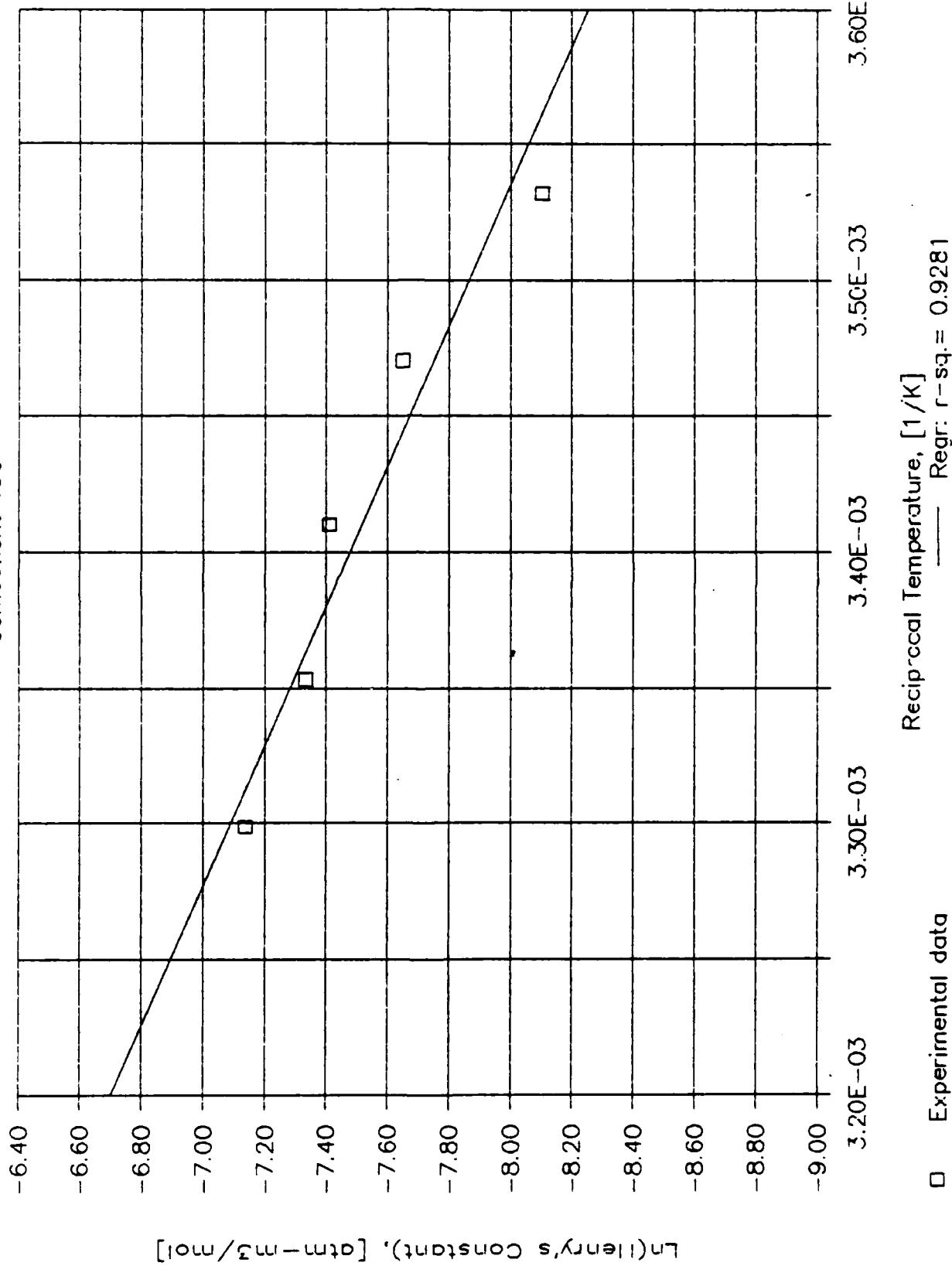
SLOPE = -3.9E+03

Y-INTERCEPT = 5.7E+00

R-SQUARED = 0.9281

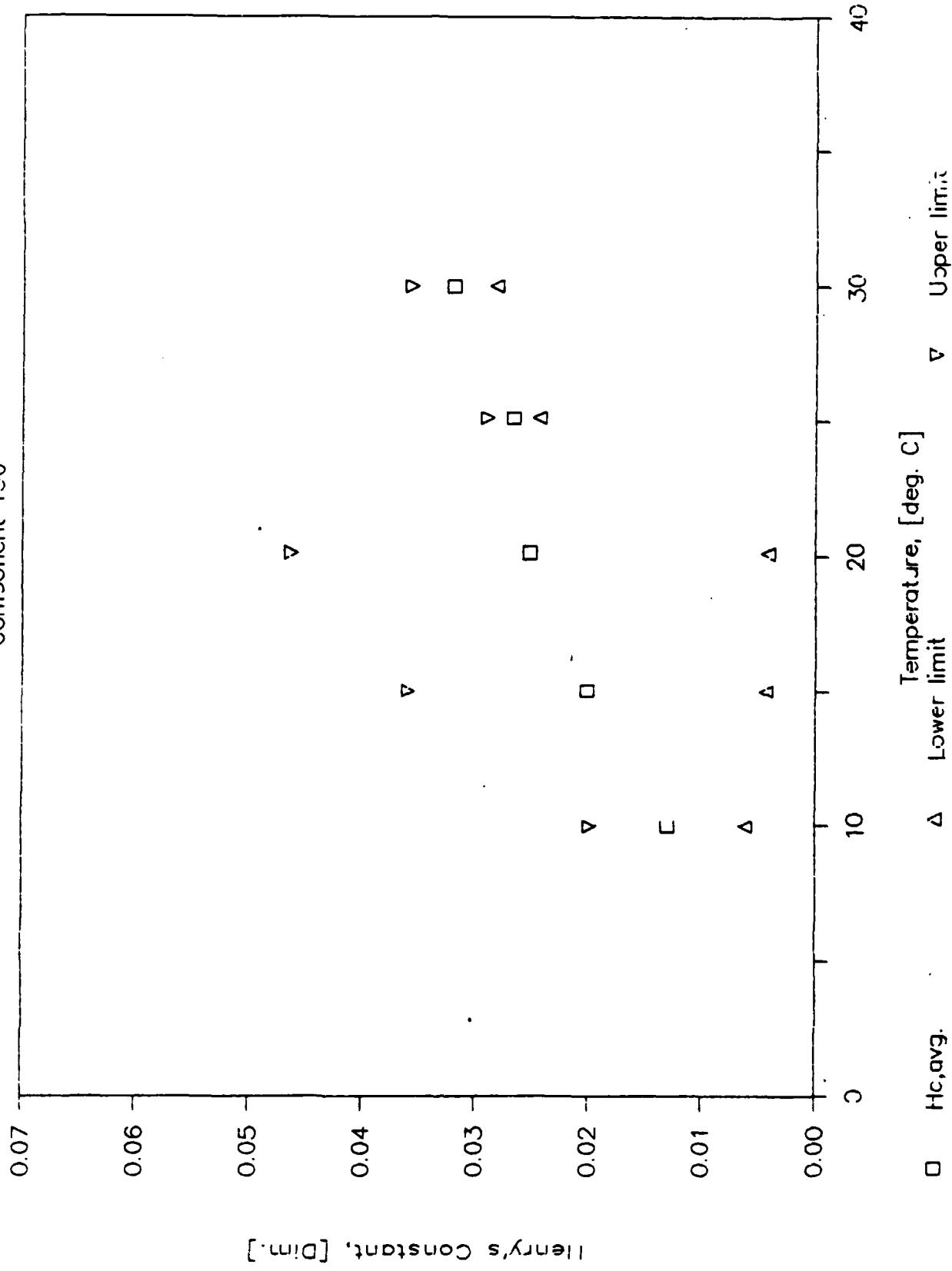
TEMPERATURE REGRESSION PLOT

Component 136



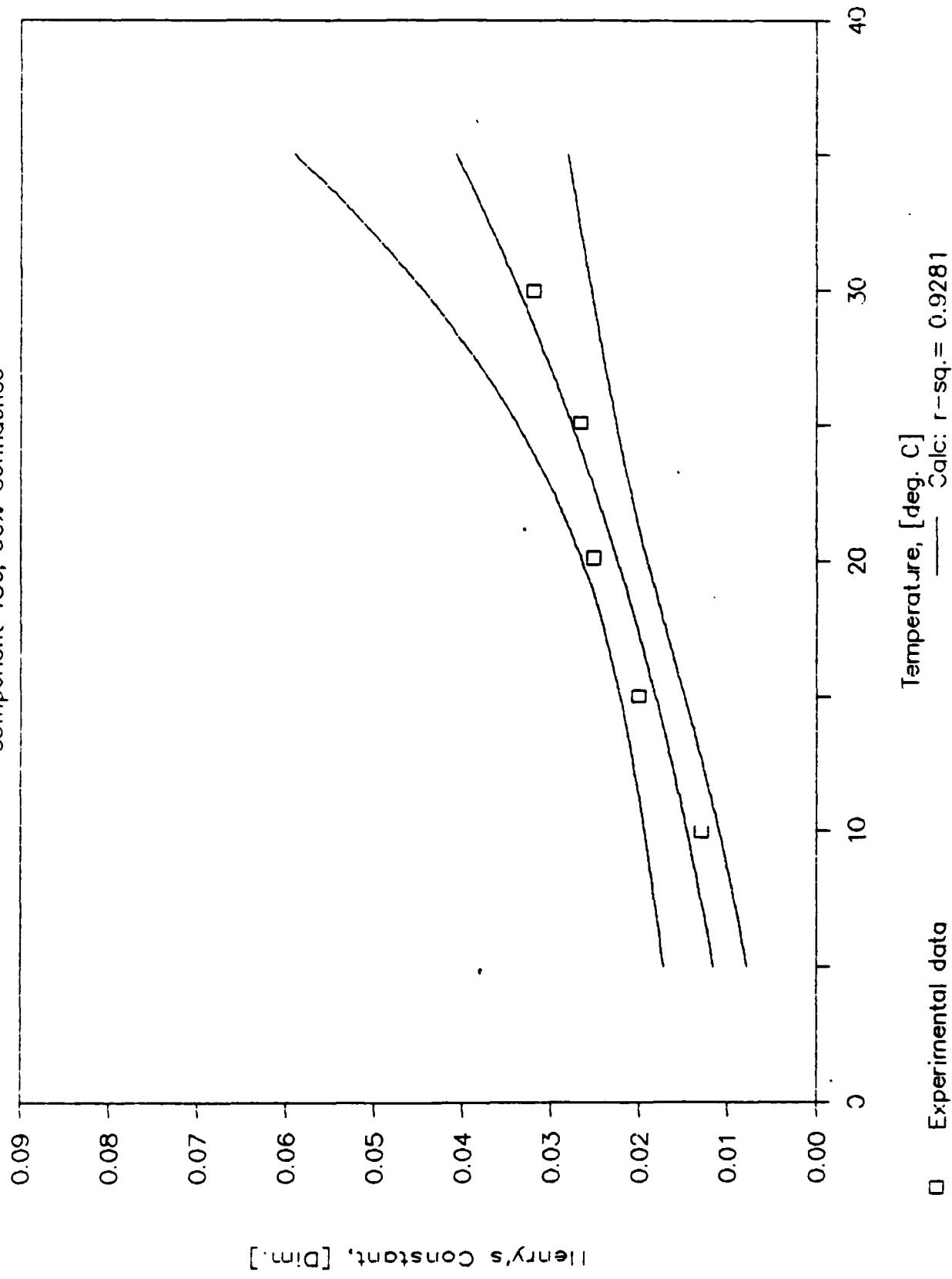
95% CONFIDENCE TEST
Component 136

283



REGRESSION CONFIDENCE TEST

Component 136, 95% Confidence



06-Nov-86

Results Summary for Component 37

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE →						
Group No.	9		9		9	
Component ID	37		37		37	
Temperature (C)	10		15		20	
Low Vol (ml)	25		25		25	
High Vol (ml)	285		285		285	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	0.6617	1.0E-25	0.8583	1.0E-25	0.9048	1.0E-25
H, avg: atm-mol/mol	853.5		1126.5		1208.1	
H, avg: atm-m3/mol	1.54E-02	1	2.03E-02	1	2.18E-02	1
H, avg: kPa-m3/mol	1.5588		2.0564		2.2054	
COV, r [std/mean]	3.41		17.22		3.09	
COV, both replic.	—	—	—	—	—	—
Observation: (1)	0.6769		0.8978		0.9007	
[atm-m3/m3] (2)	0.6388		0.6926		0.8711	
(3)	0.6849		1.0410		0.9392	
(4)	0.6464		0.8818		0.9082	
Injection: (1)	3238100		2870500		3572000	
[Peak Area] (2)	3266200		3194000		3681700	
(3)	4300400		3103100		3852300	
(4)	4485900		3748700		3947100	

06-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		12		11	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		9		9	
Component ID		37		37	
Temperature (C)		25		30	
Low Vol (ml)		25		25	
High Vol (ml)		285		285	
System Vol (ml)		250		250	
H _{avg} : atm-m ³ /mol		1.0571	1.0E-25	1.2767	1.0E-25
H _{avg} : atm-mol/mol		1435.5		1762.8	
H _{avg} : atm-m ³ /mol		2.59E-02	1	3.18E-02	1
H _{avg} : kPa-m ³ /mol		2.6285		3.2188	
COV, r [std/mean]		2.67		0.89	
COV, both replic.		—	—	—	—
Observation: (1)		1.0695		1.2895	
[atm-m ³ /mol]	(2)	1.0895		1.2711	
	(3)	1.0251		1.2822	
	(4)	1.0442		1.2639	
Injection: (1)		5147500		2865300	
[Peak Area]	(2)	4993300		2853900	
	(3)	4985100		2391500	
	(4)	4846500		2415700	

Temperature Regression Parameters:

OF POINTS = 5

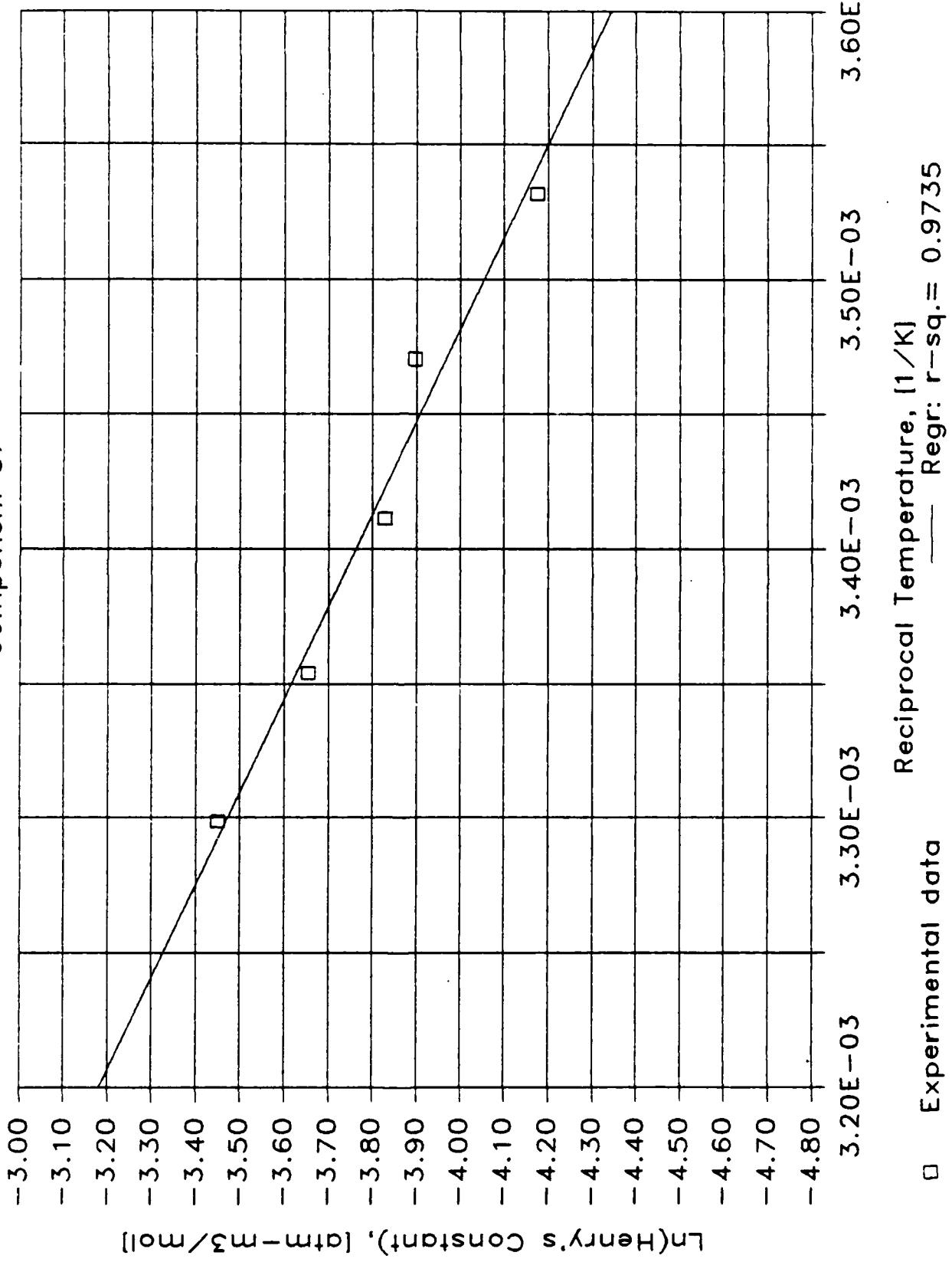
SLOPE = -2.9E+03

Y-INTERCEPT = 6.1E+00

R-SQUARED = 0.9735

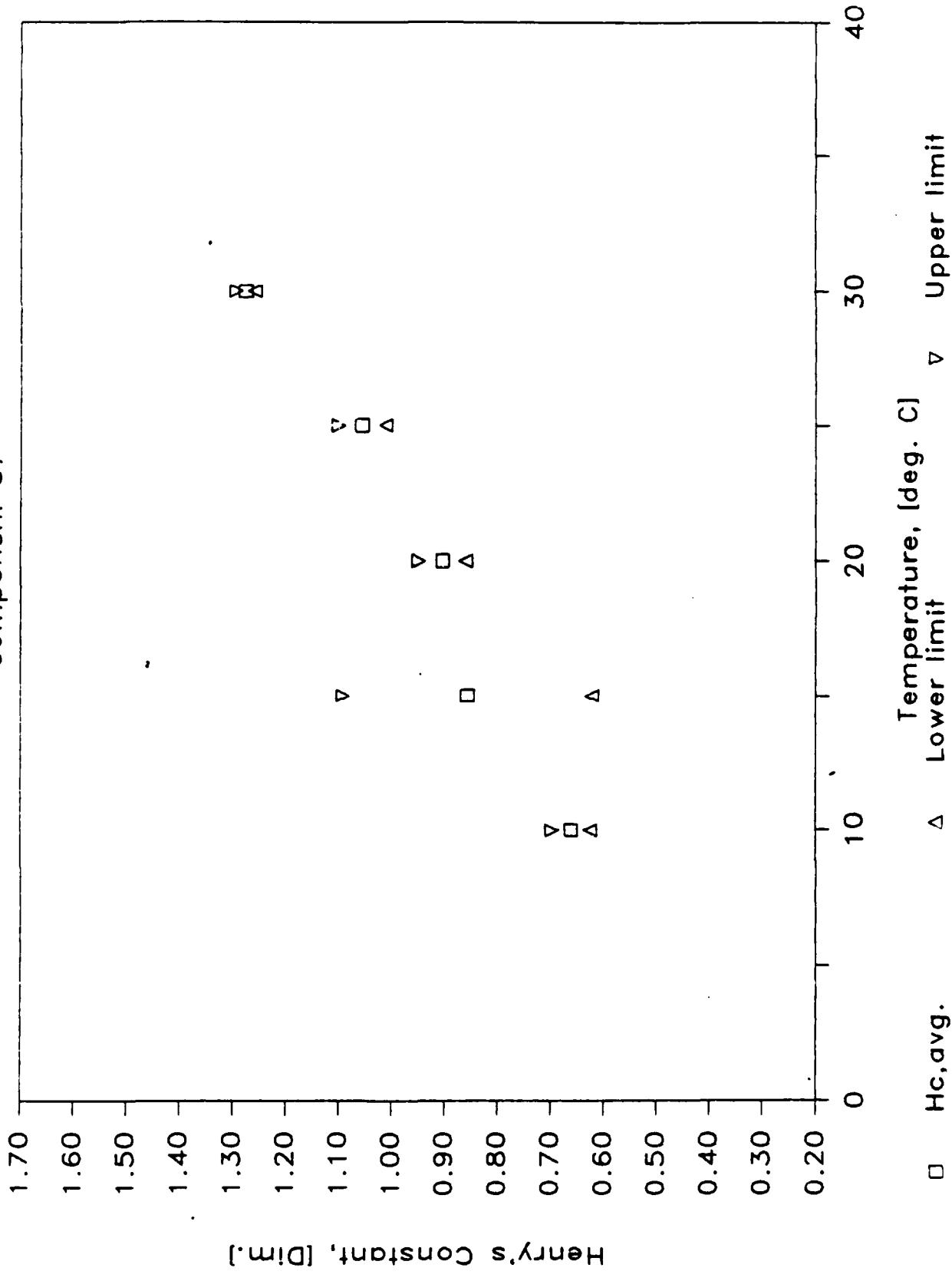
TEMPERATURE REGRESSION PLOT

Component 37



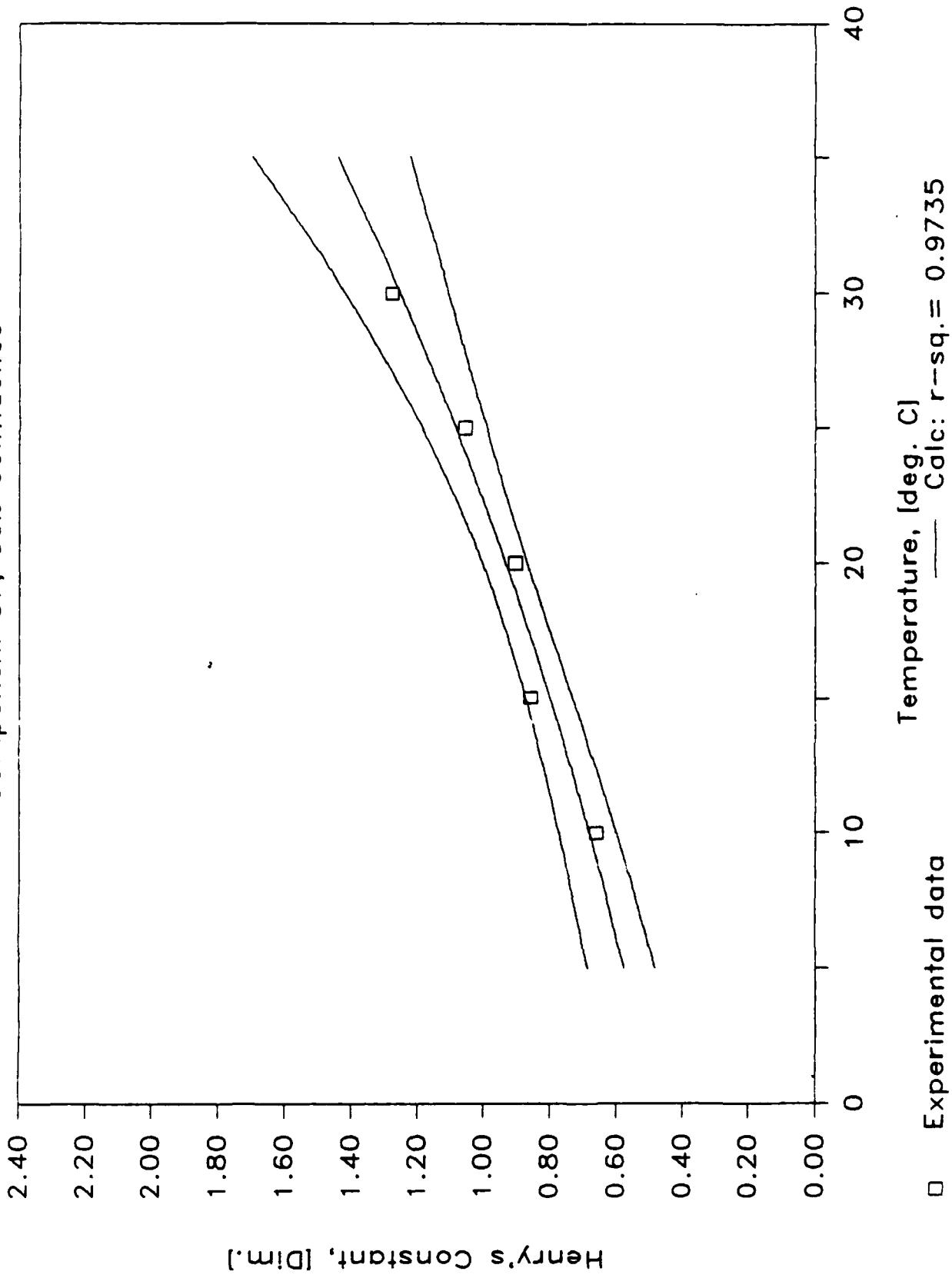
95% CONFIDENCE TEST
Component 37

288



REGRESSION CONFIDENCE TEST

Component 37, 95% Confidence



12-Aug-86

Results Summary for Component 43

RUN Number	Temperature 1		Temperature 2		Temperature 3	
	9		24		39	
REPLICATE	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	17		17		17	
Component ID	43		43		43	
Temperature (C)	10.1		15.1		19.5	
Low Vol (ml)	21		21		21	
High Vol (ml)	201		201		201	
System Vol (ml)	250		250		250	
H ₄ avg: atm-m ³ /m ³	0.0142	1.0E-25	0.0084	1.0E-25	0.0305	1.0E-25
H ₄ avg: atm-mol/mol	18.4		11.0		40.7	
H ₄ avg: atm-m ³ /mol	3.31E-04	1	1.98E-04	1	7.33E-04	1
H ₄ avg: kPa-m ³ /mol	0.0335		0.0201		0.0743	
COV, r [std/mean]	45.57		53.06		34.56	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0199		0.0055		0.0387	
[atm-m ³ /m ³] (2)	0.0198		0.0131		0.0405	
(3)	0.0087		0.0038		0.0206	
(4)	0.0086		0.0112		0.0222	
Injection: (1)	25478		34888		60686	
[Peak Area] (2)	22974		34282		52513	
(3)	201340		315460		412400	
(4)	201500		293250		406750	

12-Aug-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		25		10	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		17		17	
Component ID		43		43	
Temperature (C)		25.1		30.5	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H, avg: atm=m3/m3		0.0102	1.0E-25	0.0281	1.0E-25
H, avg: atm=mol/mol		13.9		38.8	
H, avg: atm=m3/mol		2.50E-04	1	7.00E-04	1
H, avg: kPa=m3/mol		0.0253		0.0709	
COV, r [std/mean]		86.05		56.56	
COV, both replic.		_____		_____	
Observation: (1)		0.0201		0.0228	
[atm=m3/m3] (2)		0.0147		0.0477	
(3)		0.0054		0.0099	
(4)		0.0007		0.0319	
Injection: (1)		66222		81869	
[Peak Area] (2)		57695		72903	
(3)		522440		631150	
(4)		548100		521520	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

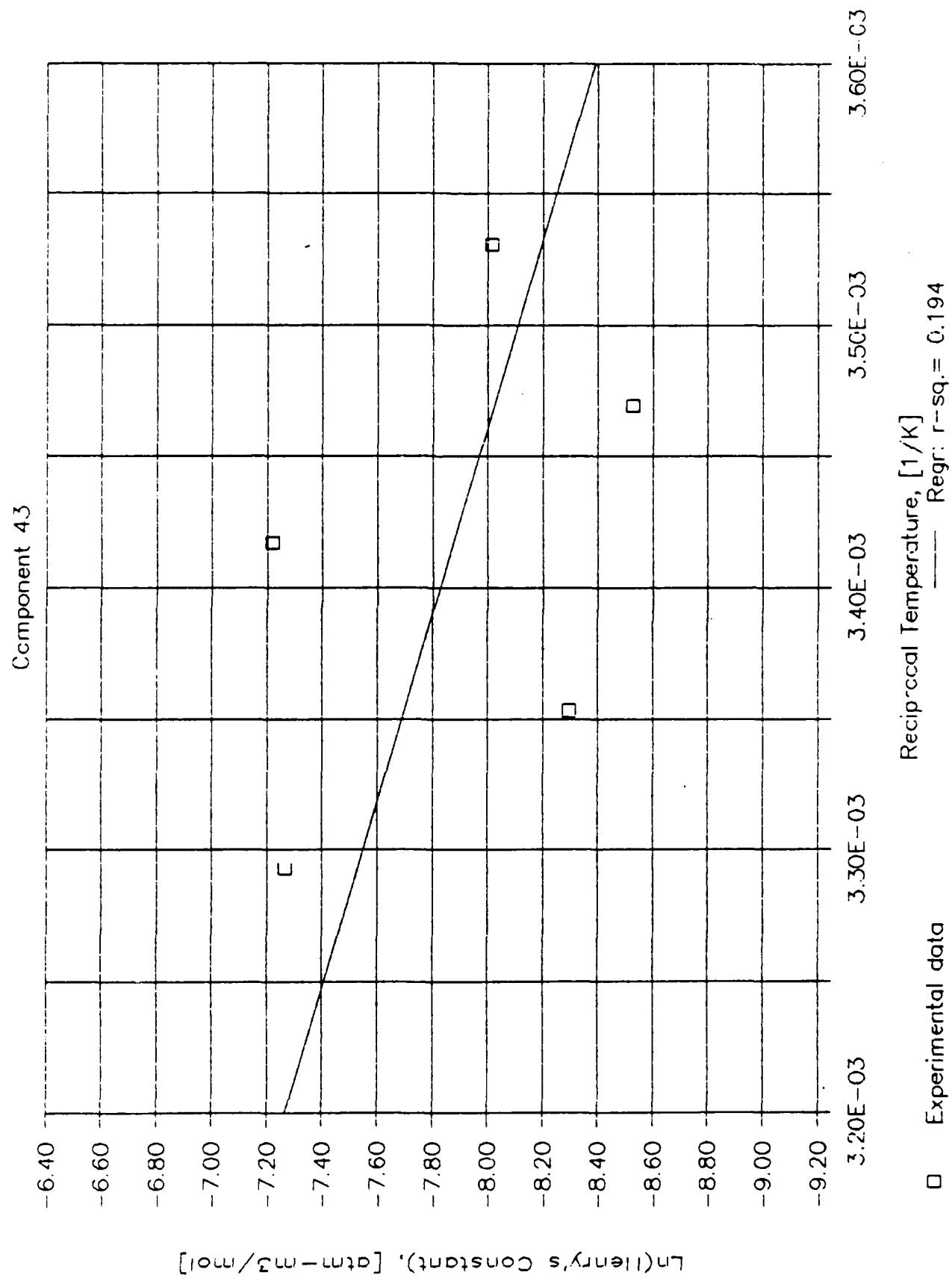
OF POINTS = 5

SLOPE = -2.8E+03

Y-INTERCEPT = 1.7E+00

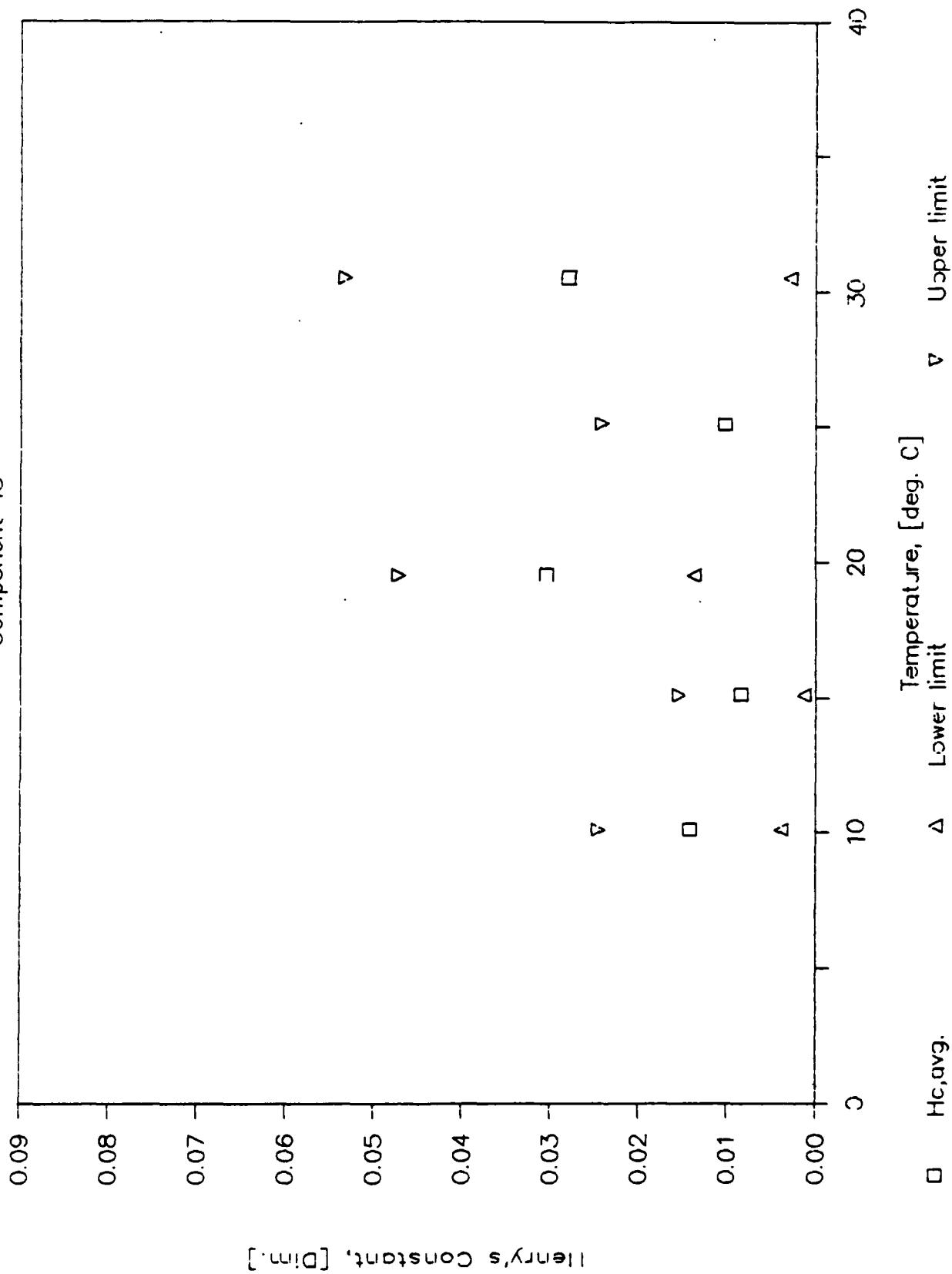
R-SQUARED = 0.1940

TEMPERATURE REGRESSION PLOT



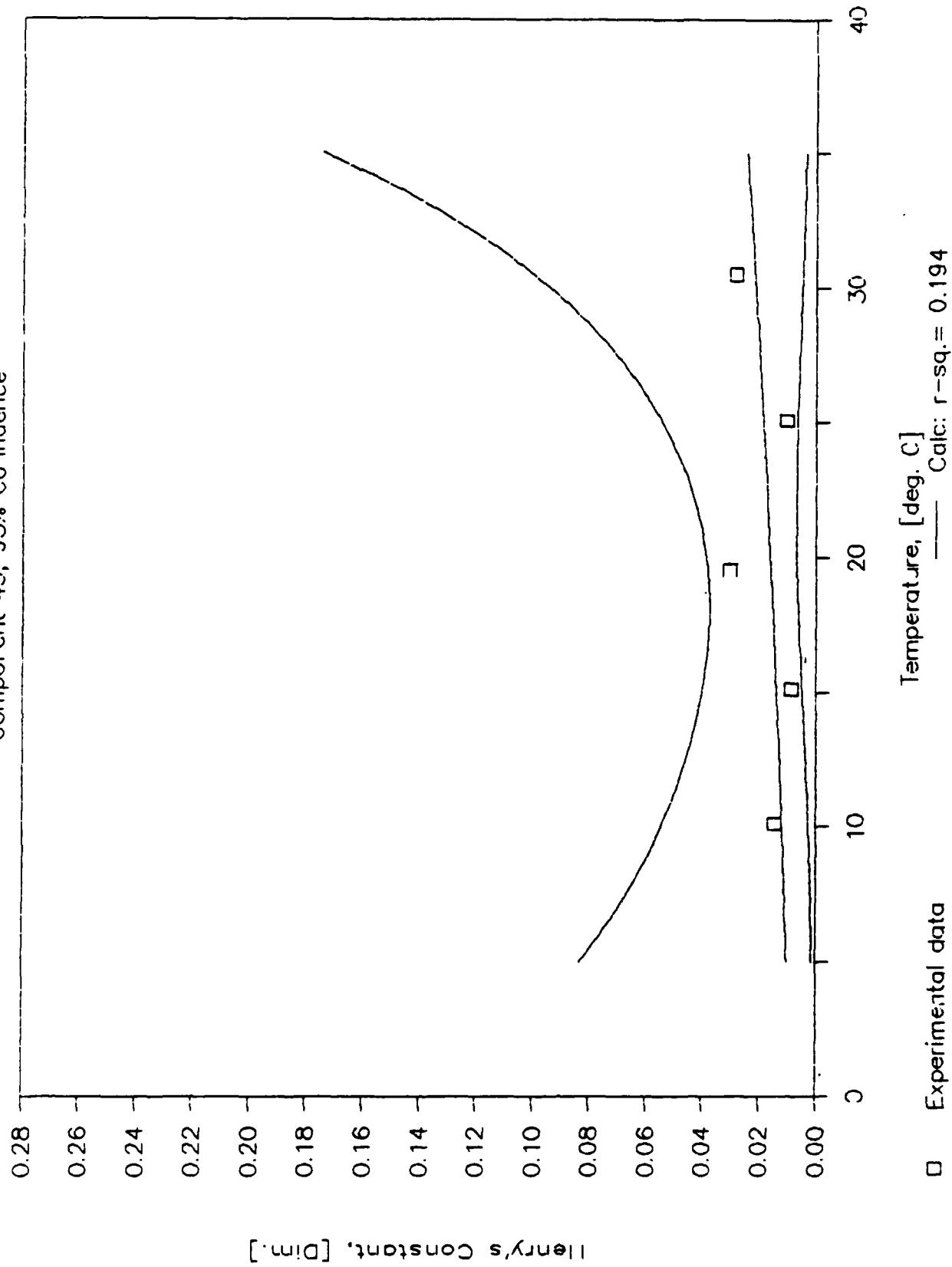
95% CONFIDENCE TEST

Component 4.3



REGRESSION CONFIDENCE TEST

Component 43, 95% Confidence



12-Aug-86

Results Summary for Component 44

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		14		28		44	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		17		17		17	
Component ID		44		44		44	
Temperature (C)		10.1		15.1		19.5	
Low Vol (ml)		21		21		21	
High Vol (ml)		201		201		201	
System Vol (ml)		250		250		250	
H, avg: atm-m3/m3		0.0526	1.0E-25	0.0535	1.0E-25	0.0792	1.0E-25
H, avg: atm-mol/mol		67.9		70.2		105.5	
H, avg: atm-m3/mol		1.22E-03	1	1.26E-03	1	1.90E-03	1
H, avg: kPa-m3/mol		0.1240		0.1281		0.1926	
COV, r [std/mean]		1.12		9.54		6.49	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.0531		0.0540		0.0842	
[atm-m3/m3] (2)		0.0521		0.0597		0.0753	
(3)		0.0532		0.0473		0.0829	
(4)		0.0522		0.0527		0.0742	
Injection: (1)		82750		104390		170130	
[Peak Area] (2)		82819		99727		168970	
(3)		508140		636940		866350	
(4)		511610		613860		910340	

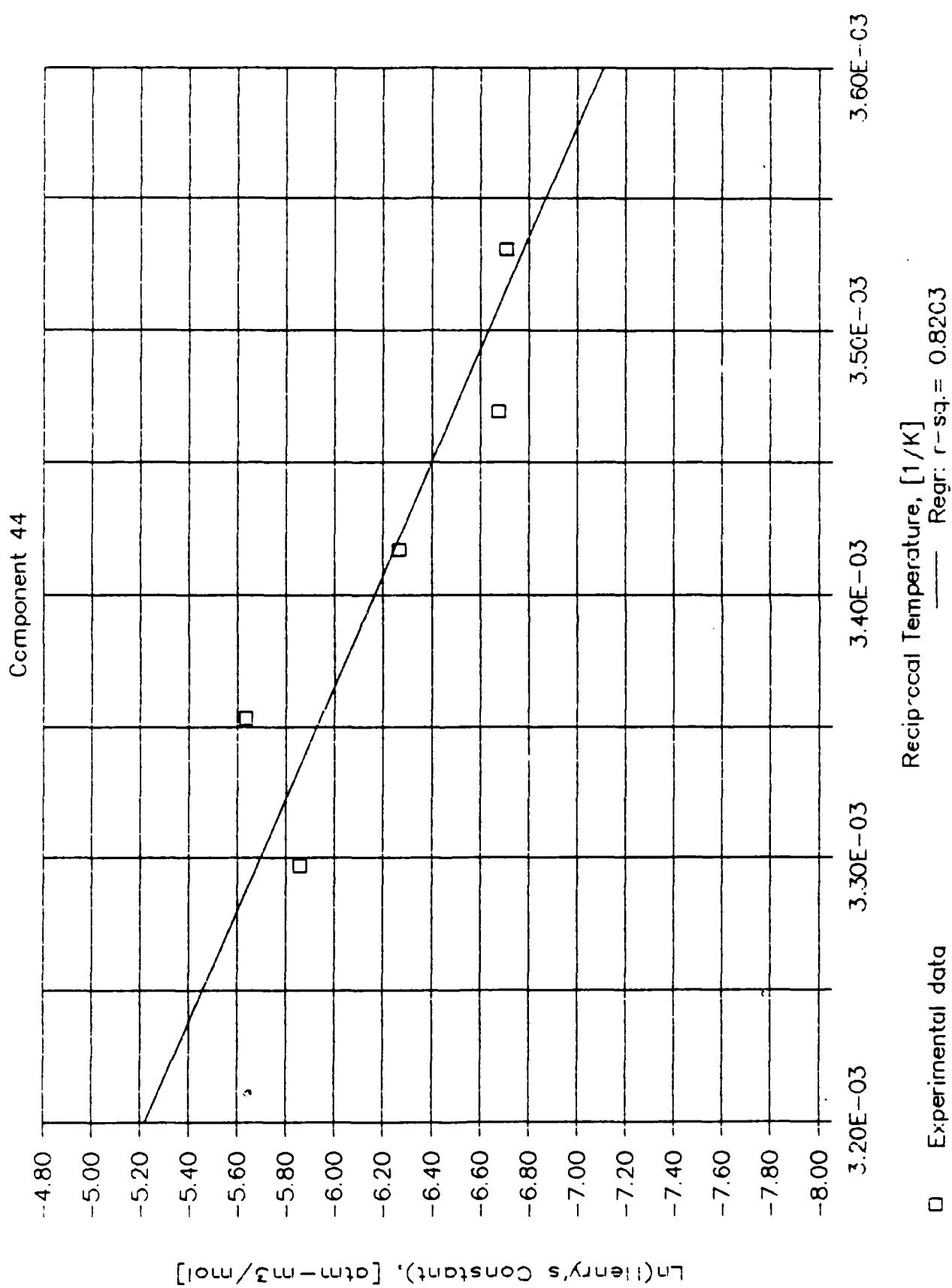
		Temperature 4		Temperature 5	
RUN Number -->		29		15	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		17		17	
Component ID		44		44	
Temperature (C)		25.1		30.15	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.1460	1.0E-25	0.1151	1.0E-25
H, avg: atm-mol/mol		198.4		158.9	
H, avg: atm-m3/mol		3.57E-03	1	2.86E-03	1
H, avg: kPa-m3/mol		0.3621		0.2901	
COV, r [std/mean]		26.57		15.31	
COV, both replic.		_____		_____	
Observation: (1)		0.1717		0.1047	
(atm-m3/mol)	(2)	0.1863		0.0963	
(3)		0.1076		0.1345	
(4)		0.1185		0.1248	
Injection: (1)		233090		184350	
[Peak Area]	(2)	179070		210840	
(3)		809300		845020	
(4)		769370		880890	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5
 SLOPE = -4.7E+03
 Y-INTERCEPT = 9.8E+00
 R-SQUARED = 0.8203

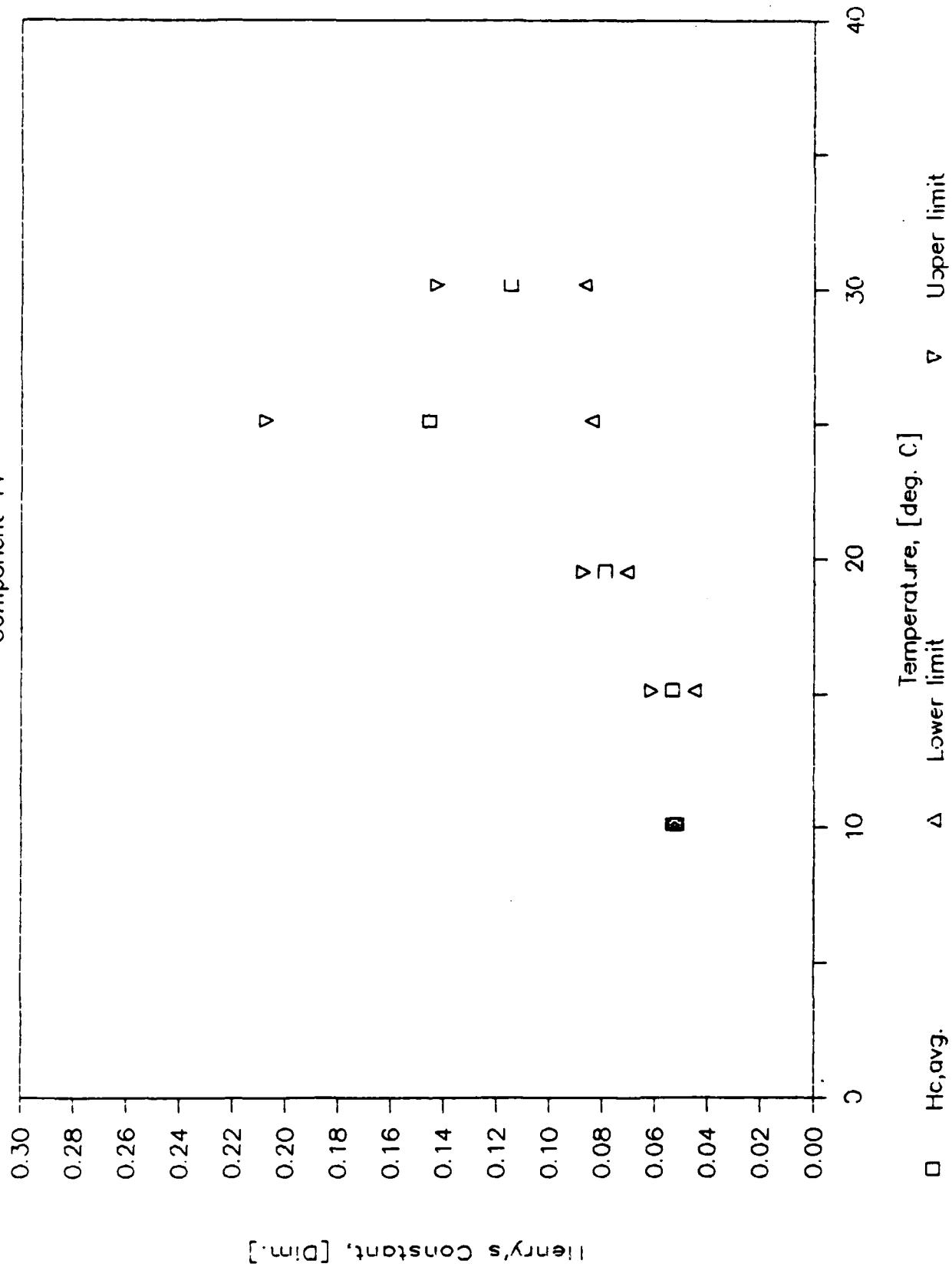
TEMPERATURE REGRESSION PLOT



95% CONFIDENCE TEST

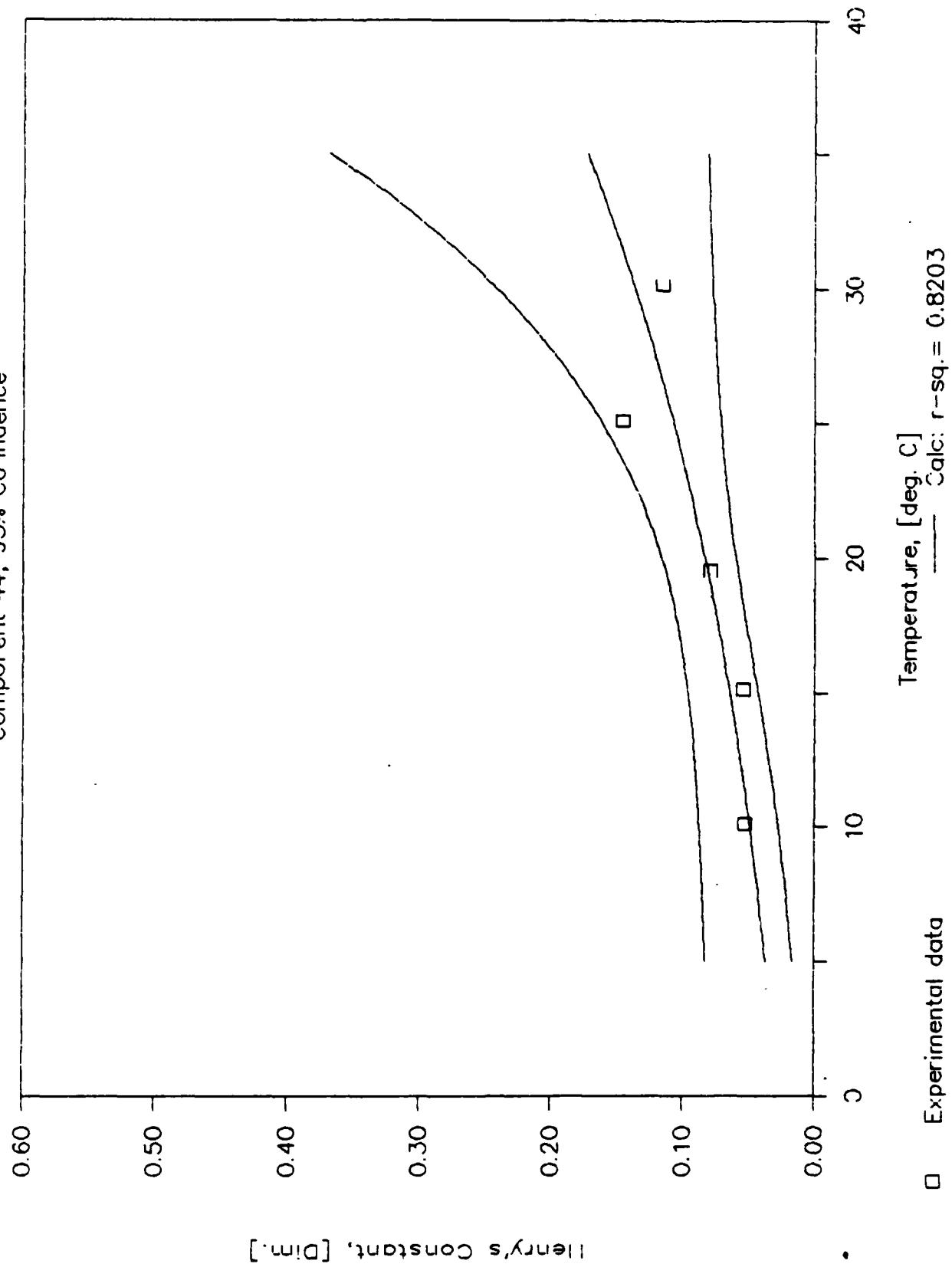
Component 44

298



REGRESSION CONFIDENCE TEST

Component 44, 95% Confidence



13-Aug-86

Results Summary for Component 45

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE —>						
Group No.	17		17		17	
Component ID	45		45		45	
Temperature (C)	10.1		15.1		19.5	
Low Vol (ml)	21		21		21	
High Vol (ml)	201		201		201	
System Vol (ml)	250		250		250	
H, avg: atm-m3/mol	0.0163	1.0E-25	0.0192	1.0E-25	0.0430	1.0E-25
H, avg: atm-mol/mol	21.0		25.2		57.3	
H, avg: atm-m3/mol	3.78E-04	1	4.55E-04	1	1.03E-03	1
H, avg: kPa-m3/mol	0.0383		0.0461		0.1046	
COV, r [std/mean]	33.91		37.20		6.20	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0229		0.0272		0.0462	
[atm-m3/mol]	(2) 0.0176		0.0229		0.0423	
(3) 0.0147		0.0153		0.0436		
(4) 0.0098		0.0114		0.0398		
Injection: (1)	53259		72470		110860	
[Peak Area]	(2) 49525		65405		108820	
(3) 410040		538410		713530		
(4) 429430		558140		733410		

13-Aug-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	35	20	No. 1	No. 2
REPLICATE →	No. 1	No. 2	No. 1	No. 2
Group No.	17		17	
Component ID	45		45	
Temperature (C)	25.1		30.15	
Low Vol (ml)	21		21	
High Vol (ml)	201		201	
System Vol (ml)	250		250	
H ₄ avg: atm-m ³ /m ³	0.0483	1.0E-25	0.0612	1.0E-25
H ₄ avg: atm-mol/mol	65.6		84.5	
H ₄ avg: atm-m ³ /mol	1.18E-03	1	1.52E-03	1
H ₄ avg: kPa-m ³ /mol	0.1197		0.1542	
COV, r [std/mm]n	2.72		4.22	
COV, both replic.	—		—	
Observation: (1)	0.0496		0.0595	
[atm-m ³ /m ³] (2)	0.0474		0.0638	
(3)	0.0491		0.0585	
(4)	0.0469		0.0628	
Injection: (1)	127970		158860	
[Peak Area] (2)	127550		157860	
(3)	804470		935680	
(4)	816920		910360	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

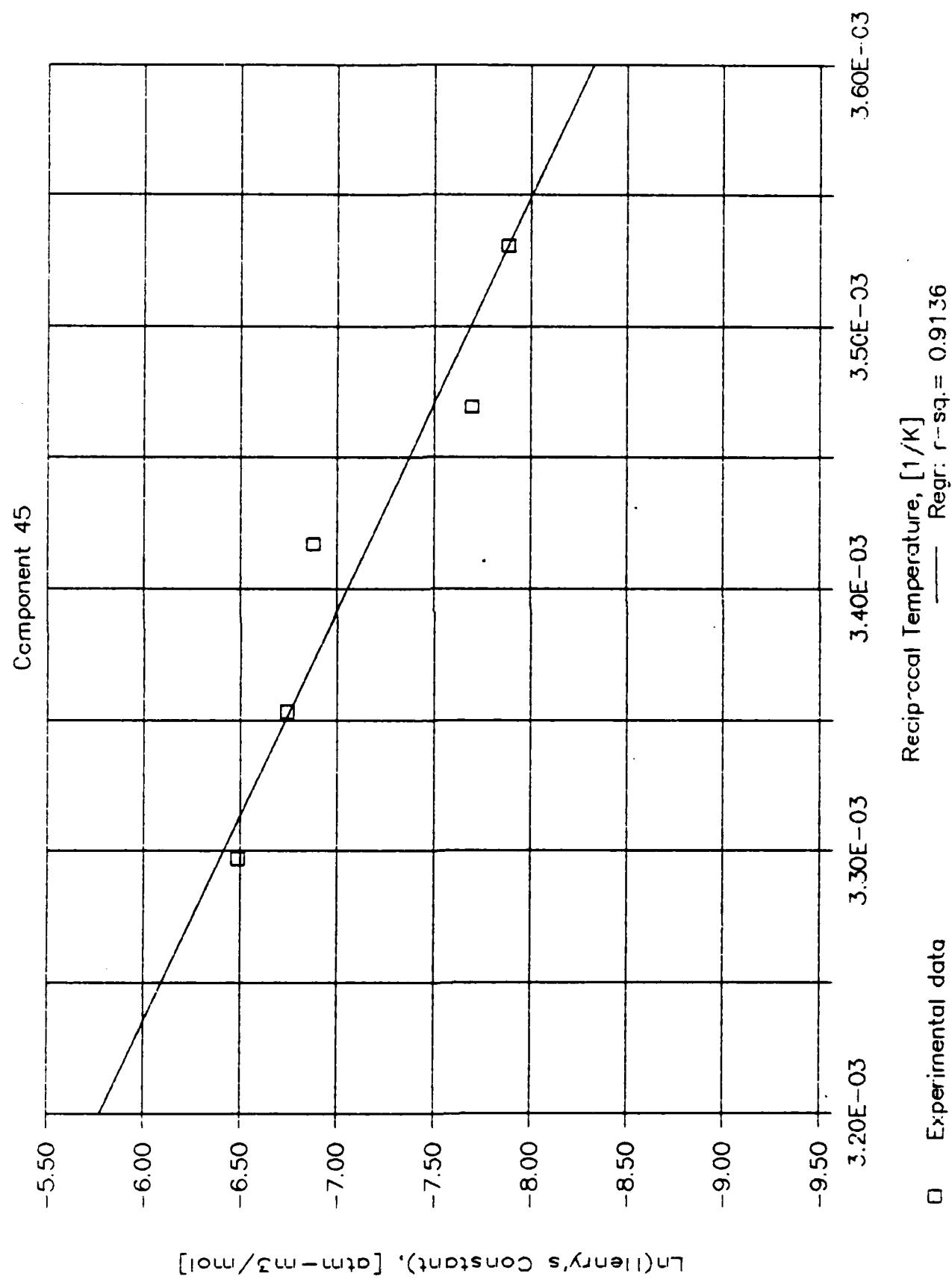
OF POINTS = 5

SLOPE = -6.4E+03

Y-INTERCEPT = 1.5E+01

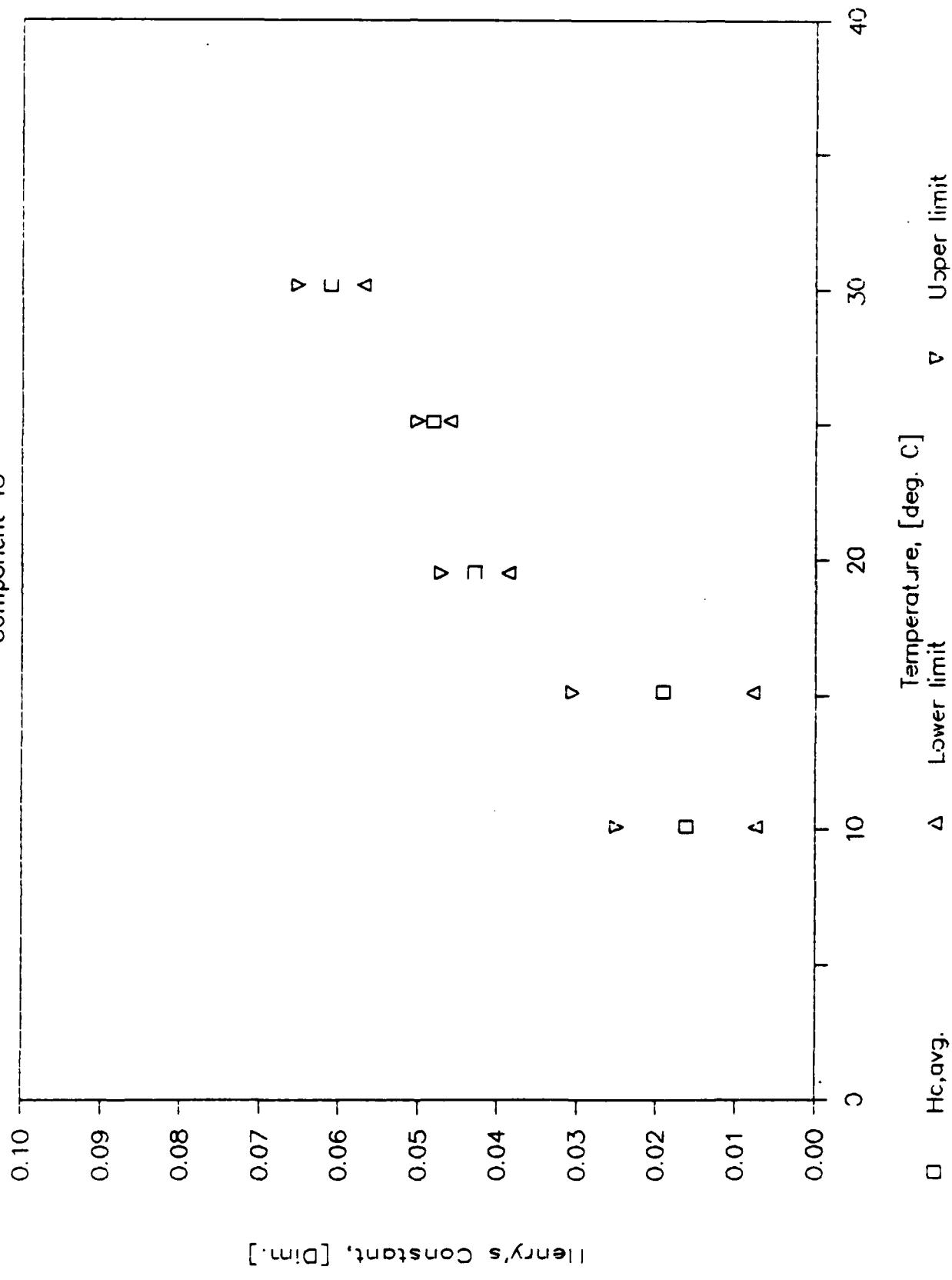
R-SQUARED = 0.9136

TEMPERATURE REGRESSION PLOT



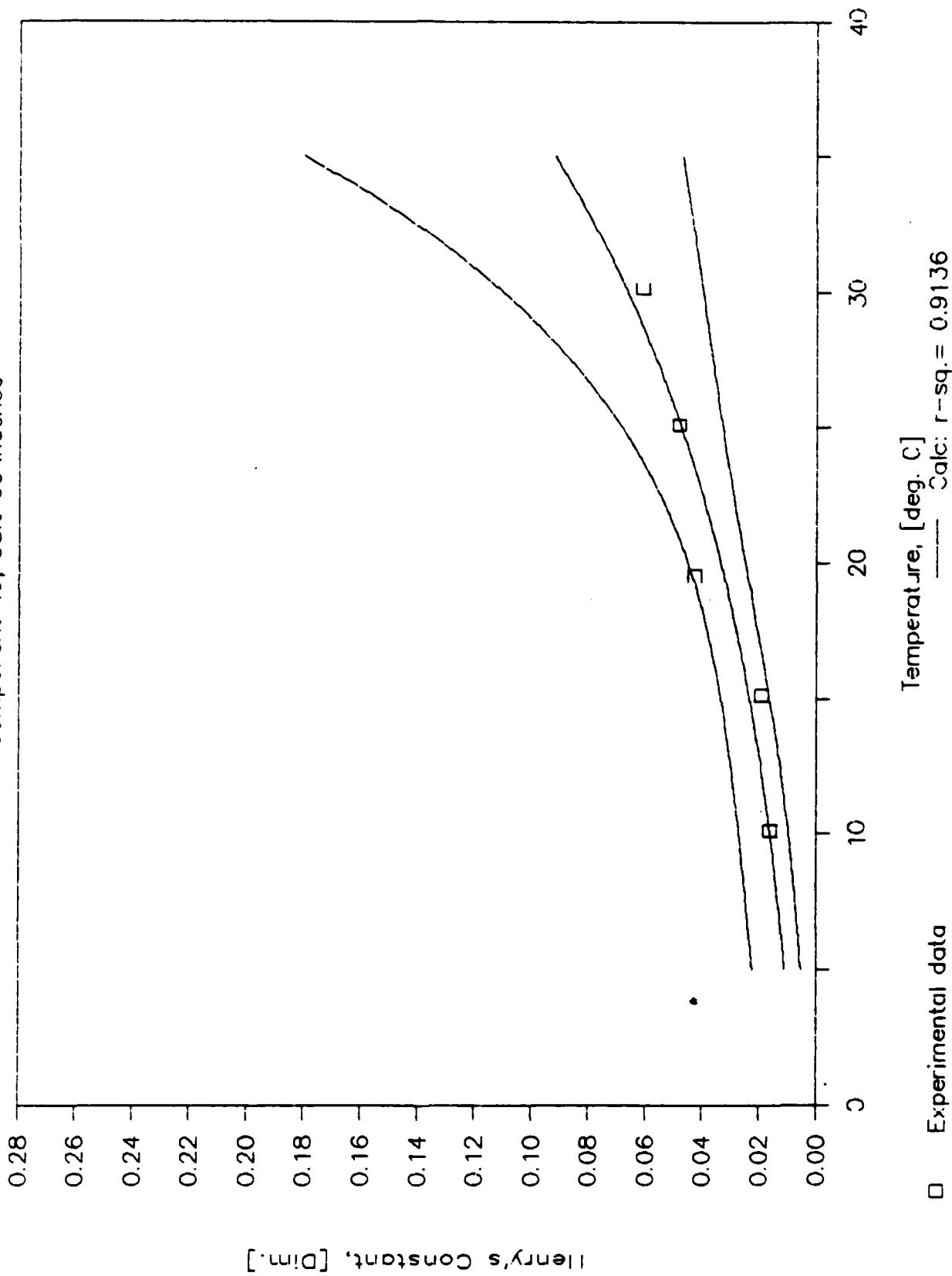
95% CONFIDENCE TEST

Component 45



REGRESSION CONFIDENCE TEST

Component 45, 95% Confidence



04-Nov-86

Results Summary for Component 46

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE —>						
Group No.	18		18		18	
Component ID	46		46		46	
Temperature (C)	10.7		15		20.2	
Low Vol (ml)	30		30		30	
High Vol (ml)	210		210		210	
System Vol (ml)	250		250		250	
H _v avg: atm=m3/m3	0.0553	1.0E-25	0.0446	1.0E-25	0.0759	1.0E-25
H _v avg: atm=mol/mol	71.5		58.5		101.5	
H _v avg: atm=m3/mol	1.29E-03	1	1.05E-03	1	1.83E-03	1
H _v avg: kPa=m3/mol	0.1305		0.1068		0.1852	
COV, r [std/mean]	39.03		51.33		7.21	
COV, both replic.	—		—		—	
Observation: (1)	0.0678		0.0486		0.0711	
[atm=m3/m3] (2)	0.0788		0.0732		0.0713	
(3)	0.0328		0.0181		0.0806	
(4)	0.0418		0.0385		0.0808	
Injection: (1)	70189		88227		121130	
[Peak Area] (2)	58535		74110		125440	
(3)	332420		459570		564880	
(4)	316050		407560		564380	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		40		35	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		18		18	
Component ID		46		46	
Temperature (C)		25.2		30	
Low Vol (ml)		30		30	
High Vol (ml)		210		210	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.0786	1.0E-25	0.1195	1.0E-25
H, avg: atm-mol/mol		106.8		164.9	
H, avg: atm-m3/mol		1.92E-03	1	2.97E-03	1
H, avg: kPa-m3/mol		0.1950		0.3011	
COV, r [std/mean]		8.18		21.95	
COV, both replic.		_____		_____	
Observation: (1)		0.0861		0.1031	
[atm-m3/mol] (2)		0.0739		0.0920	
(3)		0.0812		0.1480	
(4)		0.0712		0.1347	
Injection: (1)		148920		188820	
[Peak Area] (2)		145760		222290	
(3)		649520		767310	
(4)		679310		802970	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

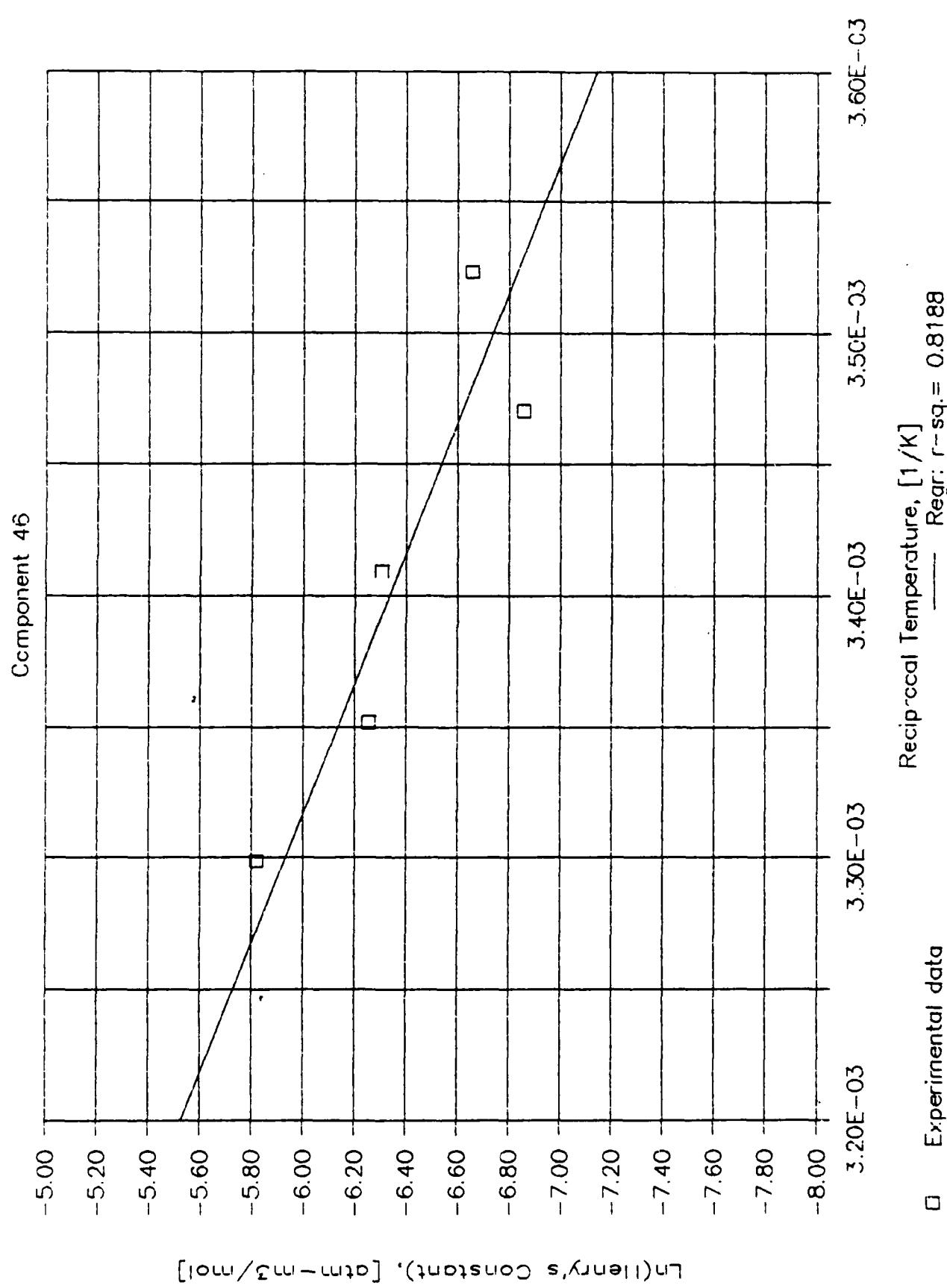
OF POINTS = 5

SLOPE = -4.0E+03

Y-INTERCEPT = 7.4E+00

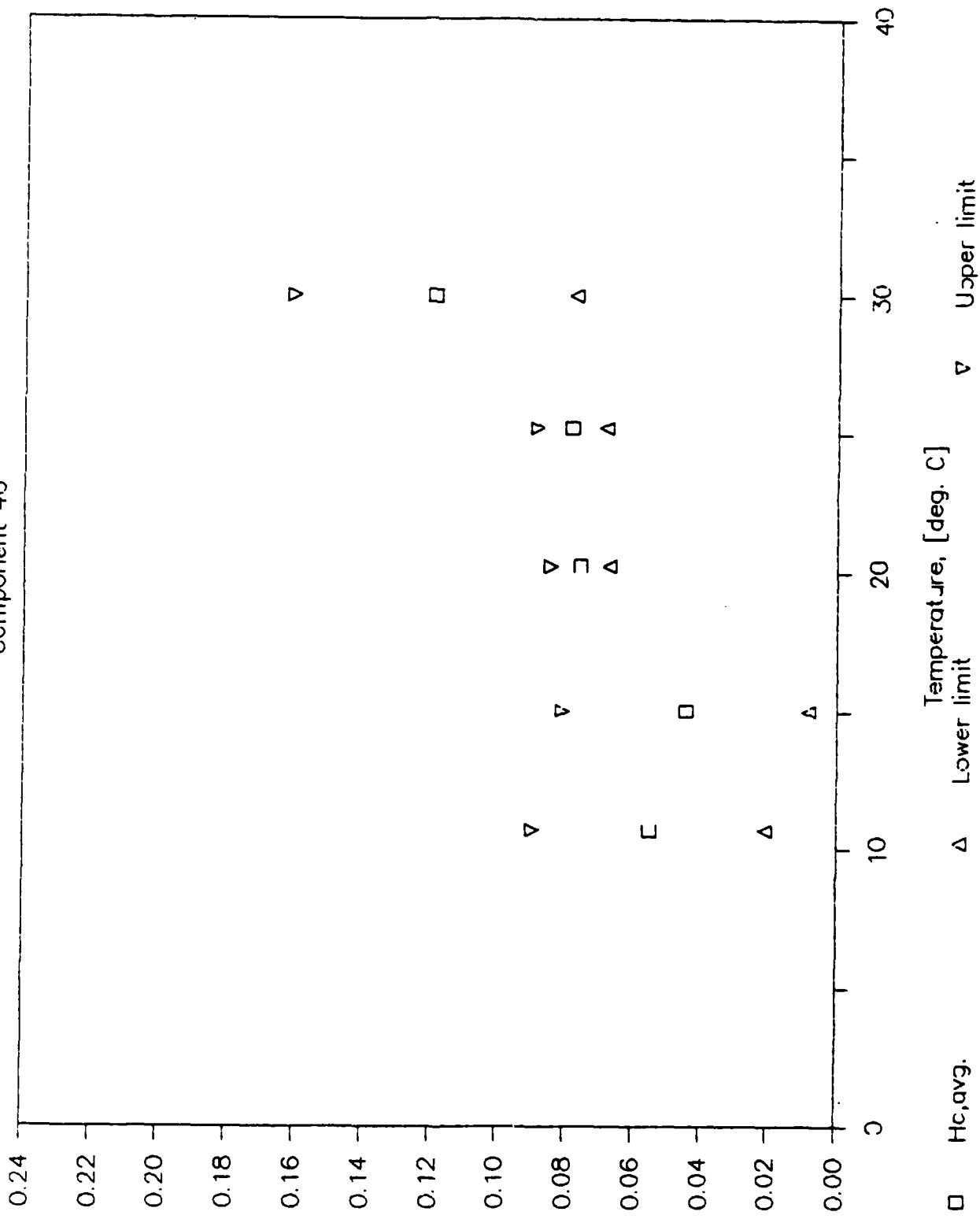
R-SQUARED = 0.8188

TEMPERATURE REGRESSION PLOT



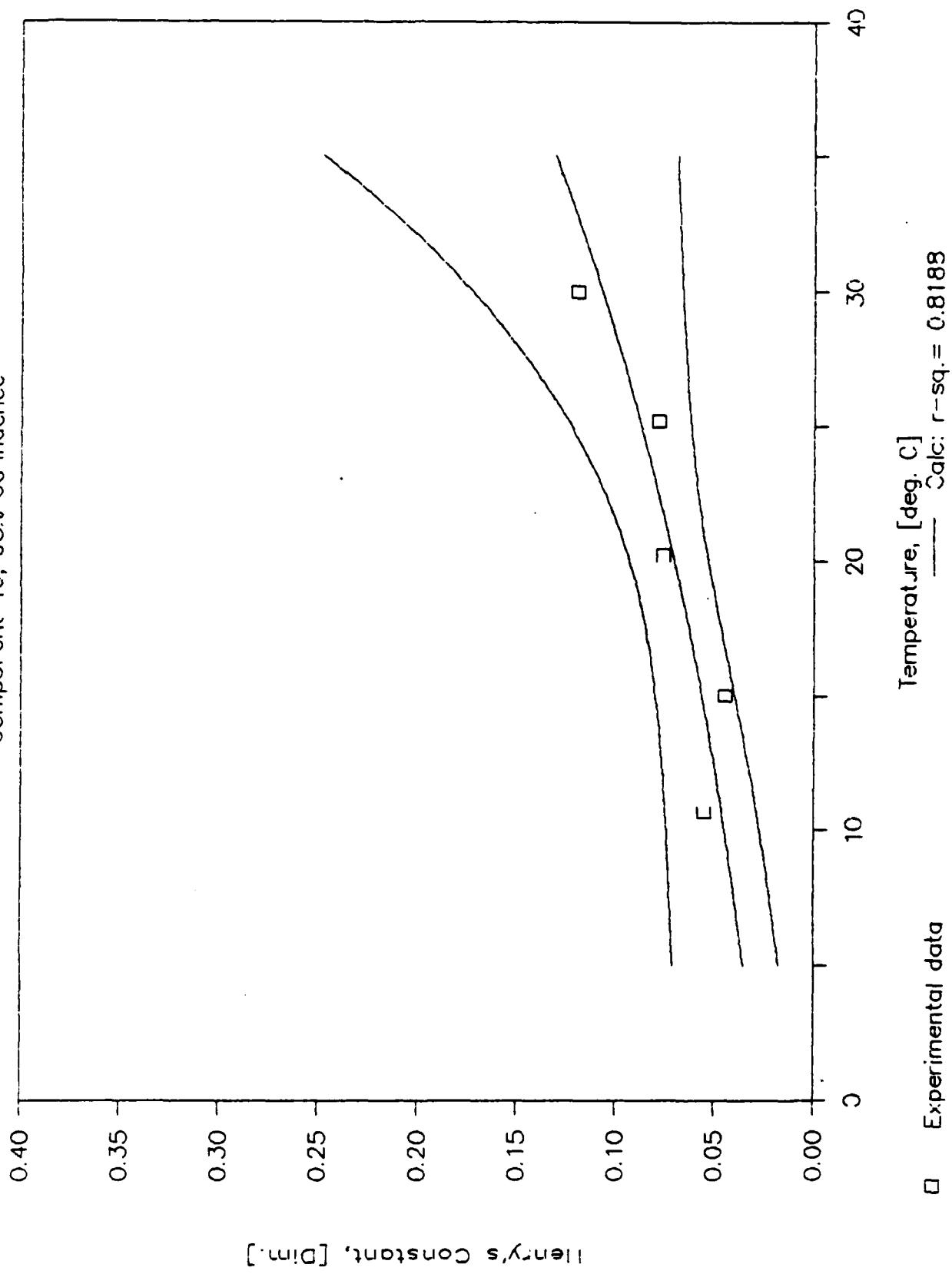
95% CONFIDENCE TEST

Component 46



REGRESSION CONFIDENCE TEST

Component 46, 95% Confidence



04-Nov-86

Results Summary for Component 47

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	30	No. 1 No. 2	45	No. 1 No. 2	25	No. 1 No. 2
REPLICATE →						
Group No.		18		18		18
Component ID		47		47		47
Temperature (C)		10.7		15		20.2
Low Vol (ml)		21		21		21
High Vol (ml)		201		201		201
System Vol (ml)		250		250		250
H, avg: atm-m3/mol	0.3560	1.0E-25		0.2850	1.0E-25	
H, avg: atm-mol/mol	460.3			374.0		562.8
H, avg: atm-m3/mol	8.29E-03	1		6.74E-03	1	1.01E-02
H, avg: kPa-m3/mol	0.8402			0.6827		1.0273
COV, r [std/mean]	22.72			12.99		19.28
COV, both replic.	_____			_____		_____
Observation: (1)	0.2649			0.3205		0.3638
[atm-m3/mol] (2)	0.3711			0.2561		0.5058
(3)	0.3300			0.3132		0.3407
(4)	0.4581			0.2500		0.4746
Injection: (1)	99857			84114		238920
[Peak Area] (2)	116350			82765		227980
(3)	261680			193110		501260
(4)	206500			225530		394260

04-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	46	31	46	31
REPLICATE →	No. 1	No. 2	No. 1	No. 2
Group No.	18		18	
Component ID	47		47	
Temperature (C)	25.2		30	
Low Vol (ml)	21		21	
High Vol (ml)	201		201	
System Vol (ml)	250		250	
H, avg: atm-m3/mol	0.2015	1.0E-25	0.1508	1.0E-25
H, avg: atm-m3/mol	273.8		208.3	
H, avg: atm-m3/mol	4.93E-03	1	3.75E-03	1
H, avg: kPa-m3/mol	0.4999		0.3802	
COV, r [std/mean]	10.40		8.17	
COV, both replic.	_____		_____	
Observation: (1)	0.2276		0.1641	
[atm-m3/mol] (2)	0.1979		0.1433	
(3)	0.2040		0.1581	
(4)	0.1766		0.1378	
Injection: (1)	150940		229280	
[Peak Area] (2)	140560		224250	
(3)	437990		818250	
(4)	479570		886390	

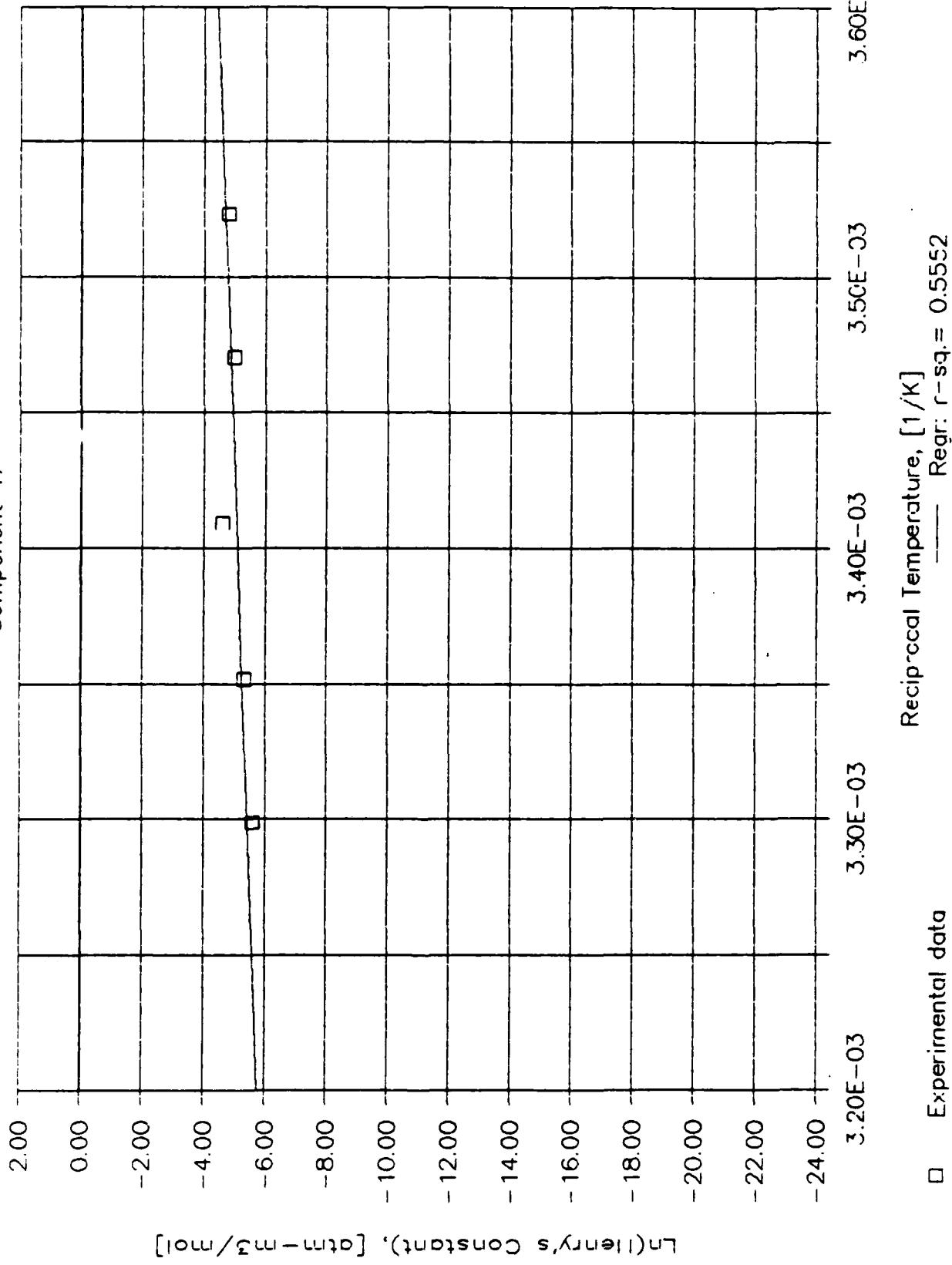
ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5
 SLOPE = 3.3E+03
 Y-INTERCEPT = -1.6E+01
 R-SQUARED = 0.5552

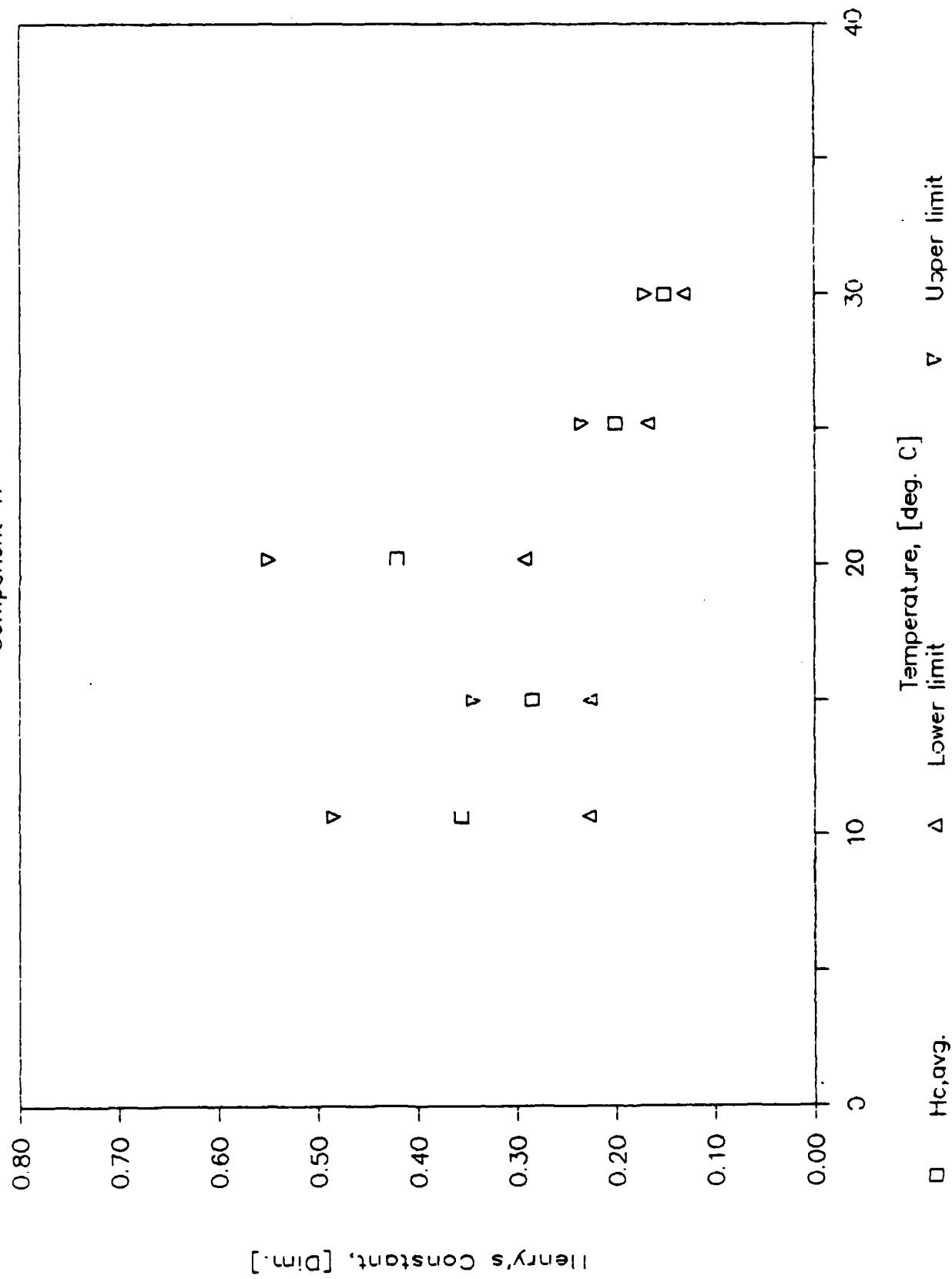
TEMPERATURE REGRESSION PLOT

Component 47



95% CONFIDENCE TEST

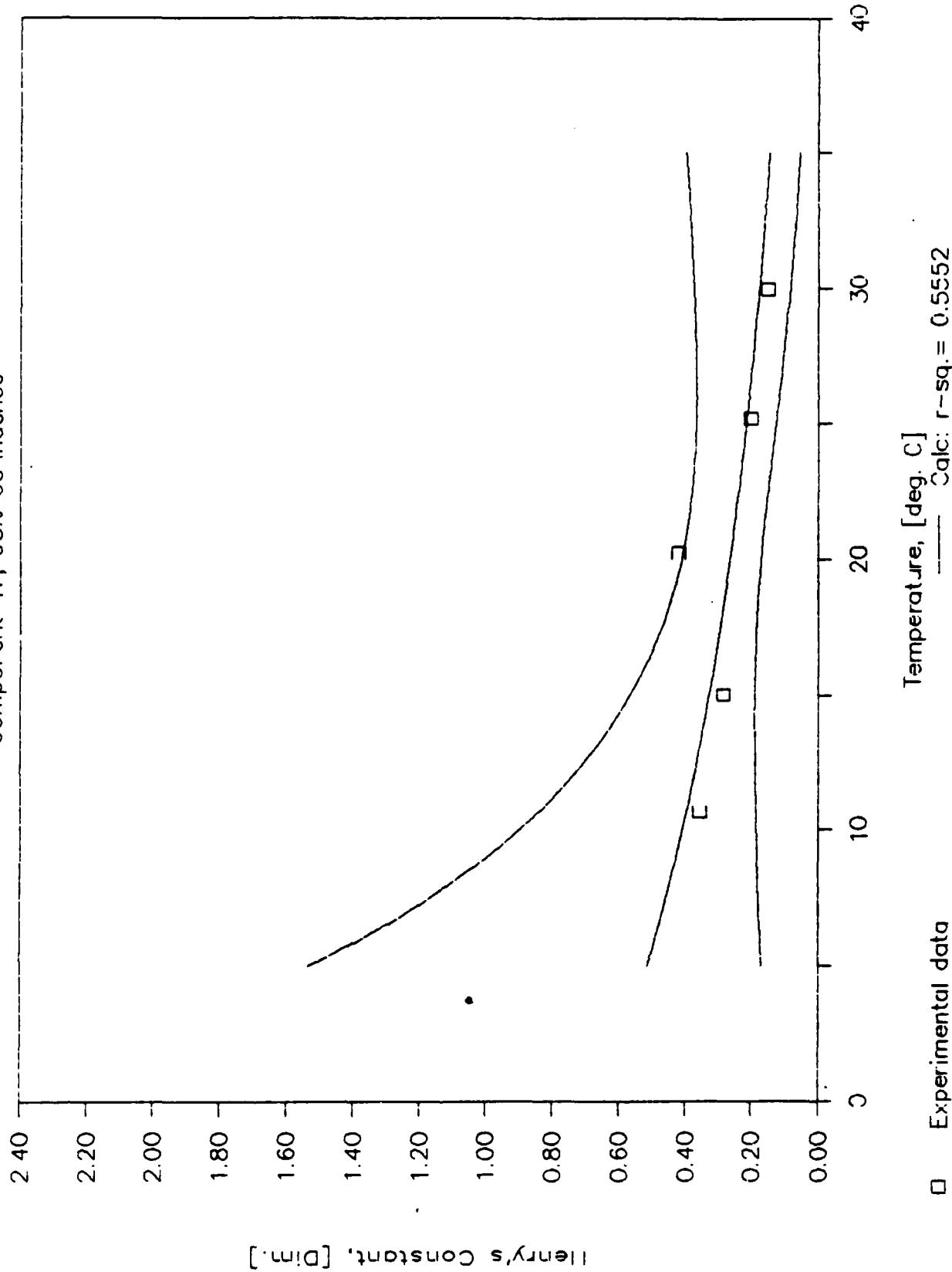
Component 47



REGRESSION CONFIDENCE TEST

Component 47, 95% Confidence

314



04-Nov-86

Results Summary for Component 49

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
	37		50		62	
REPLICATE —>	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	19		19		19	
Component ID	49		49		49	
Temperature (C)	10.2		15		19.9	
Low Vol (ml)	22		22		22	
High Vol (ml)	202		202		202	
System Vol (ml)	250		250		250	
H _{avg} : atm-m ³ /m ³	0.0995	1.0E-25	0.1228	1.0E-25	0.1553	1.0E-25
H _{avg} : atm-mol/mol	128.5		161.2		207.3	
H _{avg} : atm-m ³ /mol	2.31E-03	1	2.90E-03	1	3.73E-03	1
H _{avg} : kPa-m ³ /mol	0.2345		0.2942		0.3784	
COV, r [std/mean]	2.35		10.37		2.65	
COV, both replic.	—		—		—	
Observation: (1)	0.1018		0.1290		0.1519	
[atm-m ³ /m ³] (2)	0.1013		0.1372		0.1515	
(3)	0.0978		0.1088		0.1590	
(4)	0.0973		0.1162		0.1586	
Injections: (1)	194170		238570		262000	
[Peak Area] (2)	190410		218180		269060	
(3)	888350		966080		968120	
(4)	890840		933970		969610	

04-Nov-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	51	38	No. 1	No. 2
REPLICATE -->	No. 1	No. 2	No. 1	No. 2
Group No.	19		19	
Component ID	49		49	
Temperature (C)	25		30	
Low Vol (ml)	22		22	
High Vol (ml)	202		202	
System Vol (ml)	250		250	
H ₄ avg: atm-m ³ /m ³	0.1977	1.0E-25	0.2367	1.0E-25
H ₄ avg: atm-mol/mol	268.5		326.8	
H ₄ avg: atm-m ³ /mol	4.84E-03	1	5.89E-03	1
H ₄ avg: kPa-m ³ /mol	0.4901		0.5966	
COV, r [std/mean]	3.63		2.04	
COV, both replic.				
Observation: (1)	0.2023		0.2385	
[atm-m ³ /m ³] (2)	0.1903		0.2311	
(3)	0.2052		0.2423	
(4)	0.1930		0.2349	
Injection: (1)	360240		456690	
[Peak Area] (2)	363500		461530	
(3)	1119500		1276300	
(4)	1163300		1302900	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

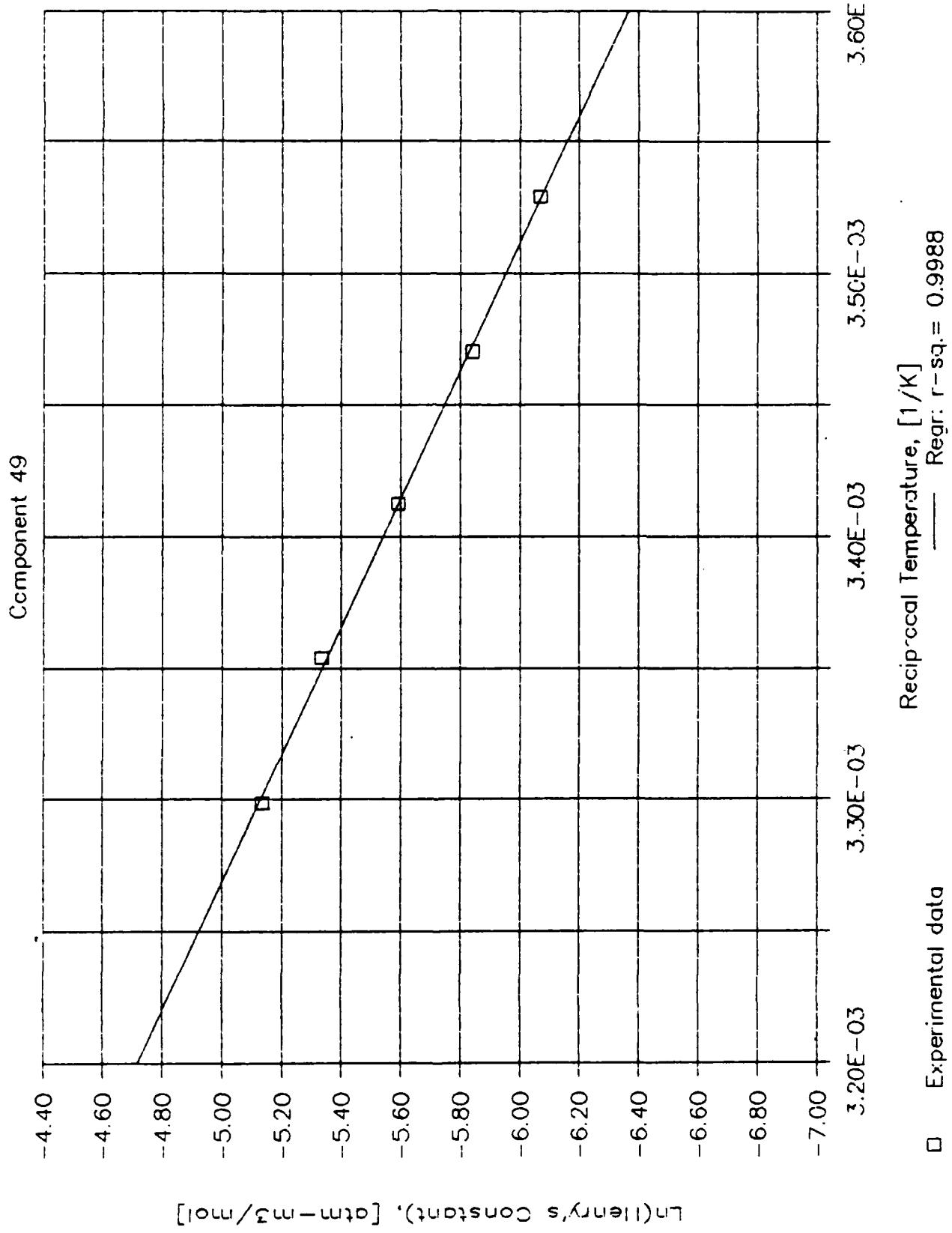
OF POINTS = 5

SLOPE = -4.1E+03

Y-INTERCEPT = 8.5E+00

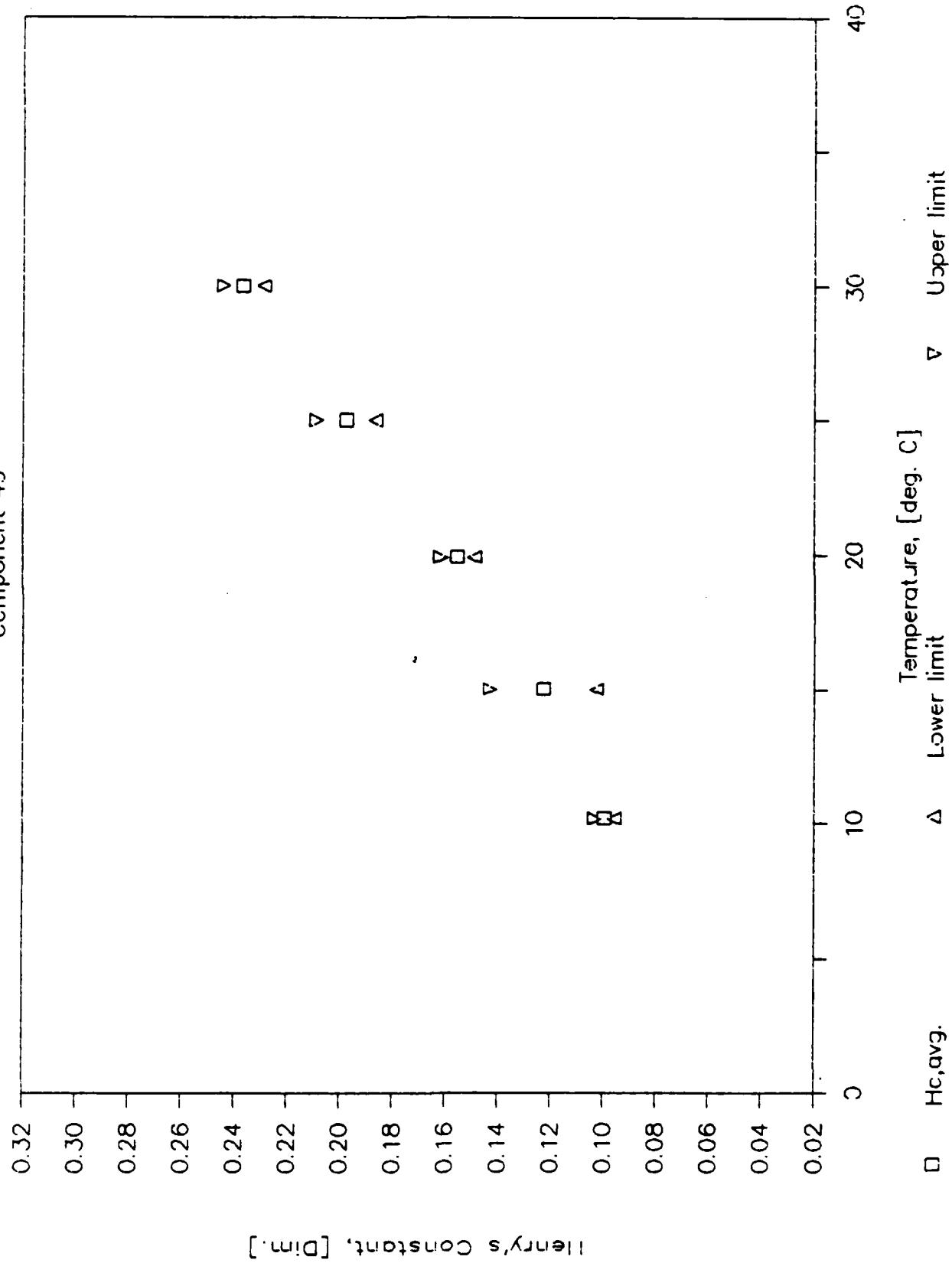
R-SQUARED = 0.9988

TEMPERATURE REGRESSION PLOT



95% CONFIDENCE TEST

Component 49

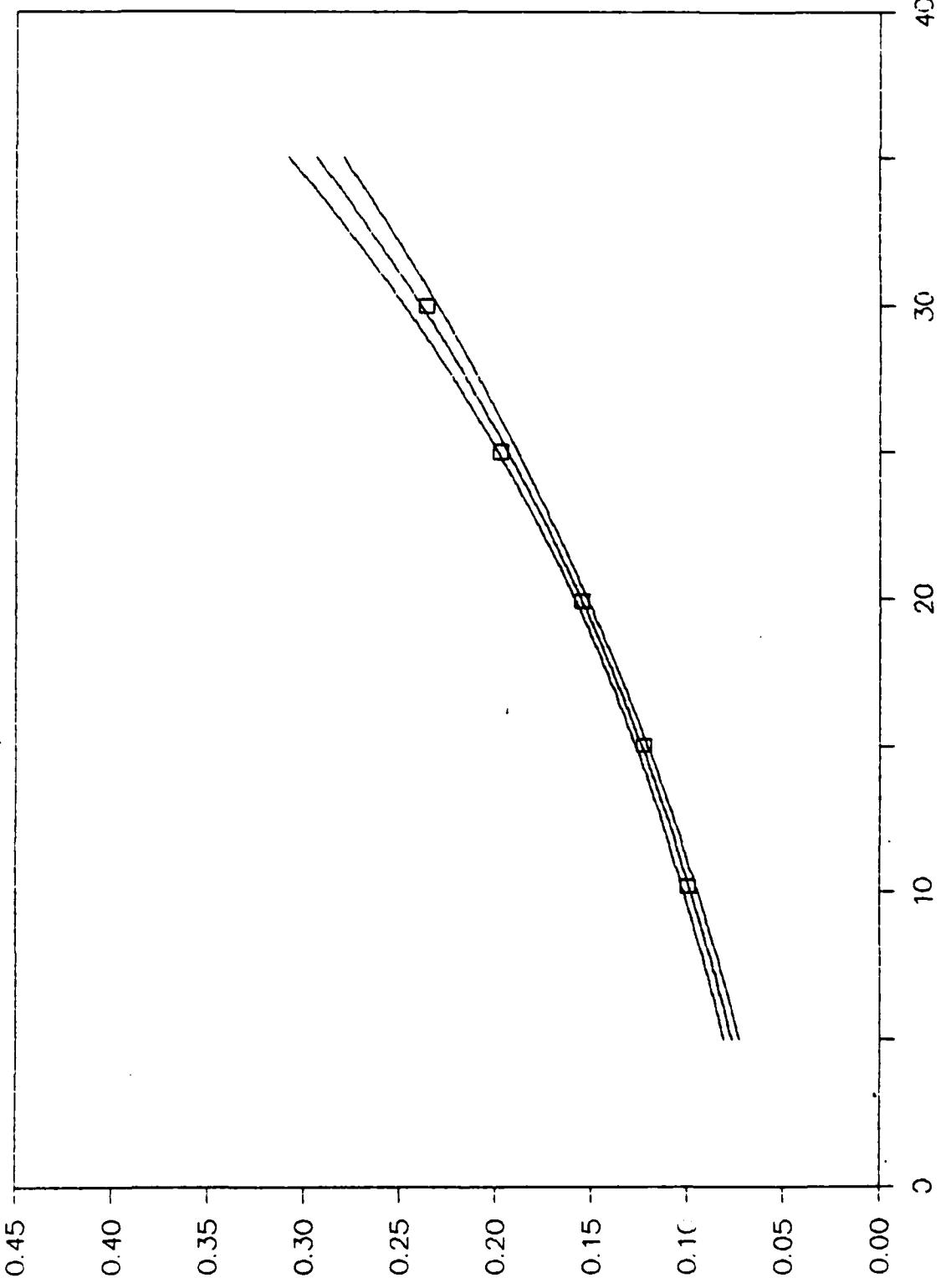


REGRESSION CONFIDENCE TEST

Component 4c, 95% Confidence

319

Henry's Constant, [Dim.]
Temperature, [deg. C]
Calc: $r^2 = 0.9988$



04-Nov-86

Results Summary for Component 50

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	19		19		19	
Component ID	50		50		50	
Temperature (C)	10.2		15		19.9	
Low Vol (ml)	22		22		22	
High Vol (ml)	202		202		202	
System Vol (ml)	250		250		250	
H _{avg} : atm-m3/m3	0.0655	1.0E-25	0.0801	1.0E-25	0.0928	1.0E-25
H _{avg} : atm-mol/mol	84.5		105.1		123.9	
H _{avg} : atm-m3/mol	1.52E-03	1	1.89E-03	1	2.23E-03	1
H _{avg} : kPa-m3/mol	0.1543		0.1919		0.2262	
COV, r [std/mean]	9.04		0.98		4.28	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0728		0.0792		0.0884	
[atm-m3/m3] (2)	0.0654		0.0805		0.0947	
(3)	0.0654		0.0797		0.0909	
(4)	0.0583		0.0810		0.0973	
Injection: (1)	533510		736390		886230	
[Peak Area] (2)	511030		738240		898130	
(3)	2840100		3783000		4336900	
(4)	2965000		3756800		4200100	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		55		42	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		19		19	
Component ID		50		50	
Temperature (C)		25		30	
Low Vol (ml)		22		22	
High Vol (ml)		202		202	
System Vol (ml)		250		250	
H _{avg} : atm=m3/m3		0.1538	1.0E-25	0.1400	1.0E-25
H _{avg} : atm=mol/mol		208.9		193.4	
H _{avg} : atm=m3/mol		3.76E-03	1	3.48E-03	1
H _{avg} : kPa=m3/mol		0.3813		0.3530	
COV, r [std/mean]		3.32		2.37	
COV, both replic.		_____		_____	
Observation: (1)		0.1530		0.1440	
[atm=m3/m3] (2)		0.1476		0.1392	
(3)		0.1600		0.1409	
(4)		0.1545		0.1361	
Injection:	(1)	1251600		1163700	
[Peak Area]	(2)	1284900		1149400	
(3)		4606400		4433100	
(4)		4701400		4519900	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

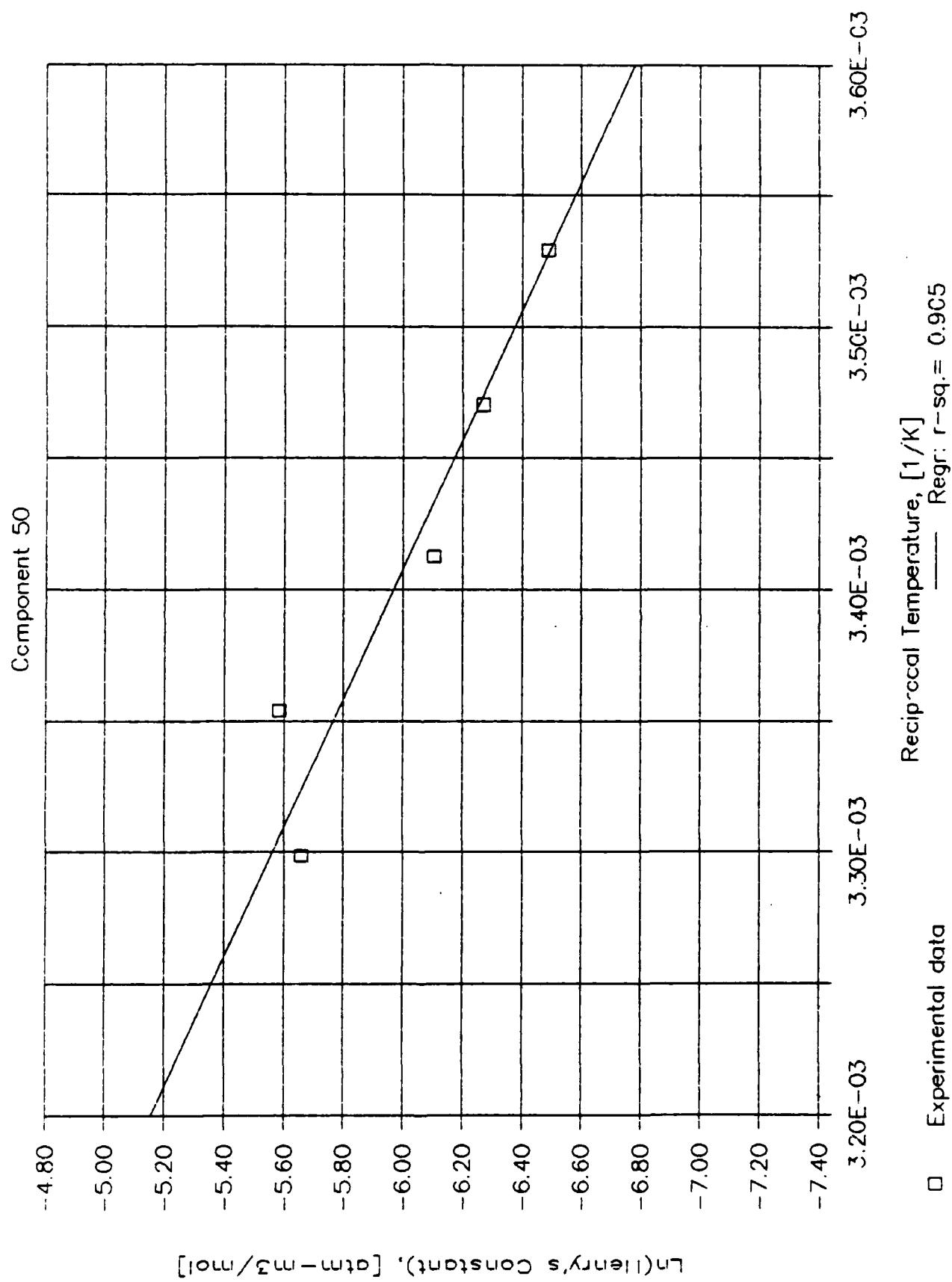
OF POINTS = 5

SLOPE = -4.1E+03

Y-INTERCEPT = 7.9E+00

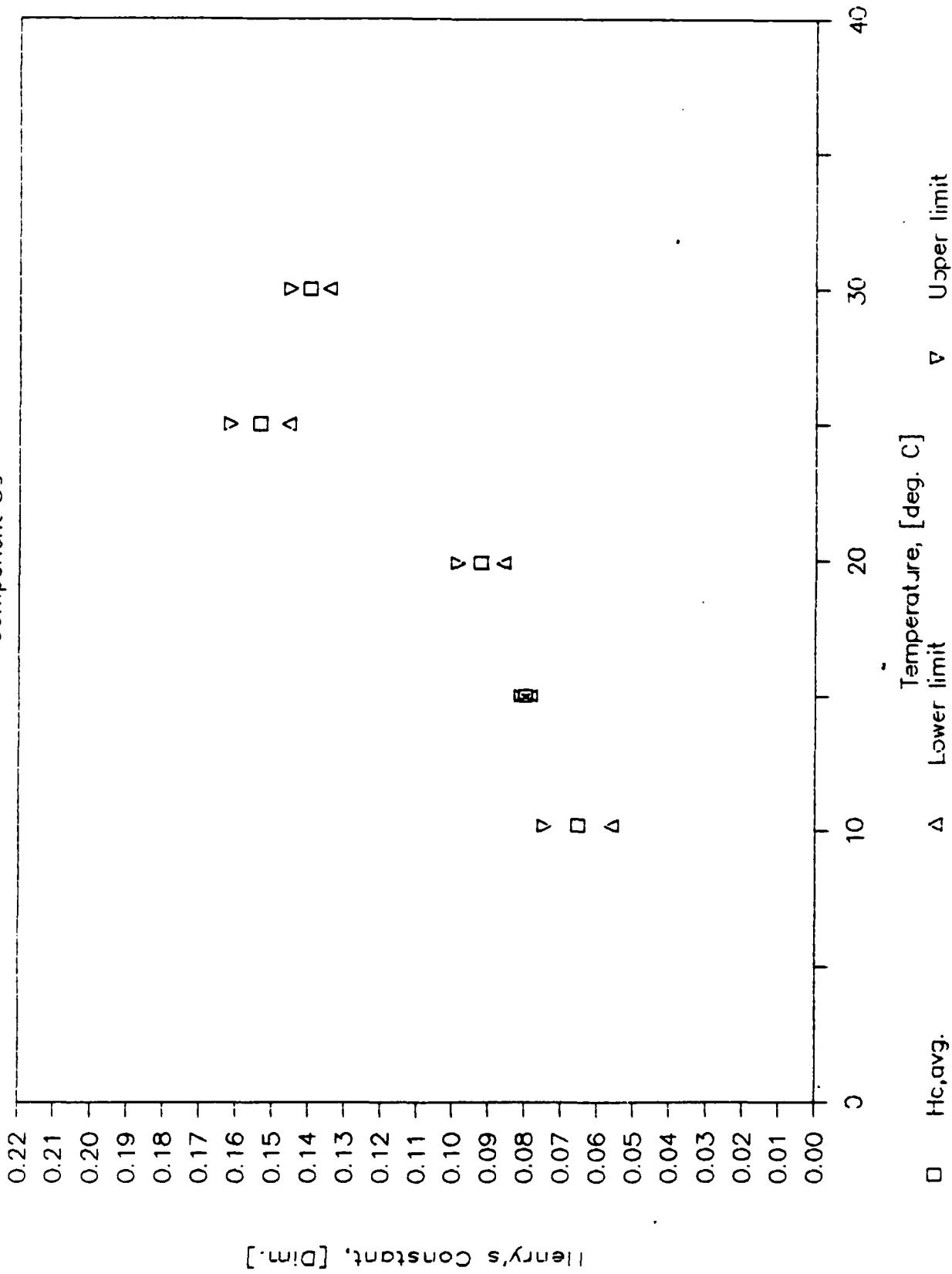
R-SQUARED = 0.9050

TEMPERATURE REGRESSION PLOT



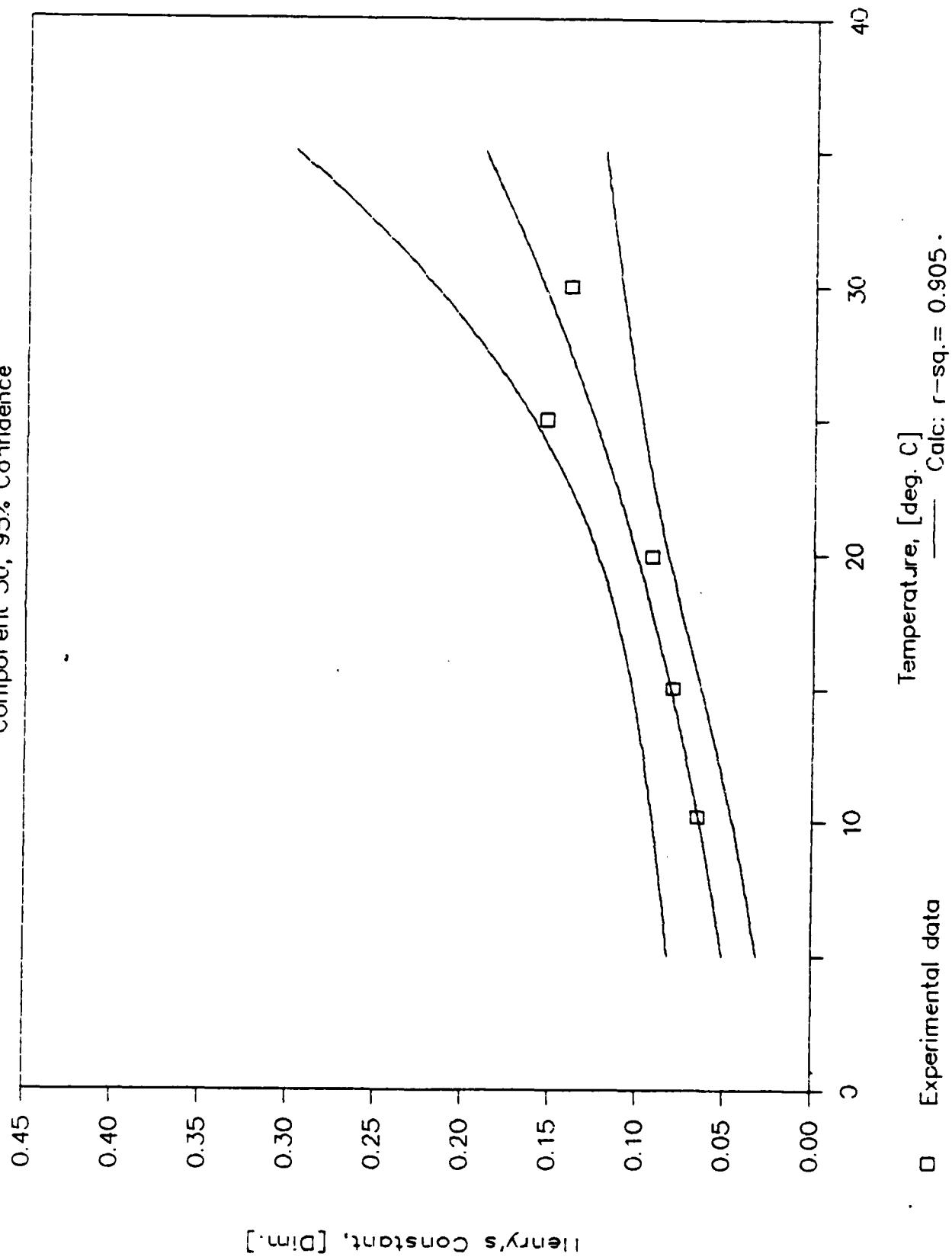
95% CONFIDENCE TEST

Component 50



REGRESSION CONFIDENCE TEST

Component 50, 95% Confidence



04-Nov-86

Results Summary for Component 51

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
REPLICATE -->						
Group No.	19		19		19	
Component ID	51		51		51	
Temperature (C)	10.2		15		19.9	
Low Vol (ml)	22		22		22	
High Vol (ml)	202		202		202	
System Vol (ml)	250		250		250	
H, avg: atm-m3/m3	6.6092	1.0E-25	9.1000	1.0E-25	10.1702	1.0E-25
H, avg: atm-mol/mol	8529.9		11943.5		13575.1	
H, avg: atm-m3/mol	1.54E-01	1	2.15E-01	1	2.45E-01	1
H, avg: kPa-m3/mol	15.5712		21.8026		24.7809	
COV, r [std/mean]	5.63		8.21		7.40	
COV, both replic.						
Observation: (1)	6.2345		8.5849		9.7805	
(atm-m3/m3) (2)	6.3524		9.8822		9.3493	
(3)	6.8564		8.3488		11.0394	
(4)	6.9936		9.5841		10.5115	
Injection: (1)	3602800		3672000		2731900	
[Peak Area] (2)	3734300		3639300		2825800	
(3)	1251100		1139200		814570	
(4)	1242100		1091600		825500	

04-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	59	47	No. 1	No. 2
REPLICATE →			No. 1	No. 2
Group No.	19		19	
Component ID	51		51	
Temperature (C)	25		30	
Low Vol (ml)	22		22	
High Vol (ml)	202		202	
System Vol (ml)	250		250	
H, avg: atm-m3/m3	13.0355	1.0E-25	12.9085	1.0E-25
H, avg: atm-mol/mol	17702.5		17824.0	
H, avg: atm-m3/mol	3.19E-01	1	3.21E-01	1
H, avg: kPa-m3/mol	32.3154		32.5372	
COV, r [std/mean]	5.60		3.00	
COV, both replic.	—		—	
Observation: (1)	12.2717		12.5670	
(atm-m3/m3) (2)	12.5795		12.5789	
(3)	13.4640		13.2374	
(4)	13.8266		13.2505	
Injection: (1)	4235400		4664300	
(Peak Area) (2)	4330400		4722500	
(3)	1188100		1300800	
(4)	1180900		1300500	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

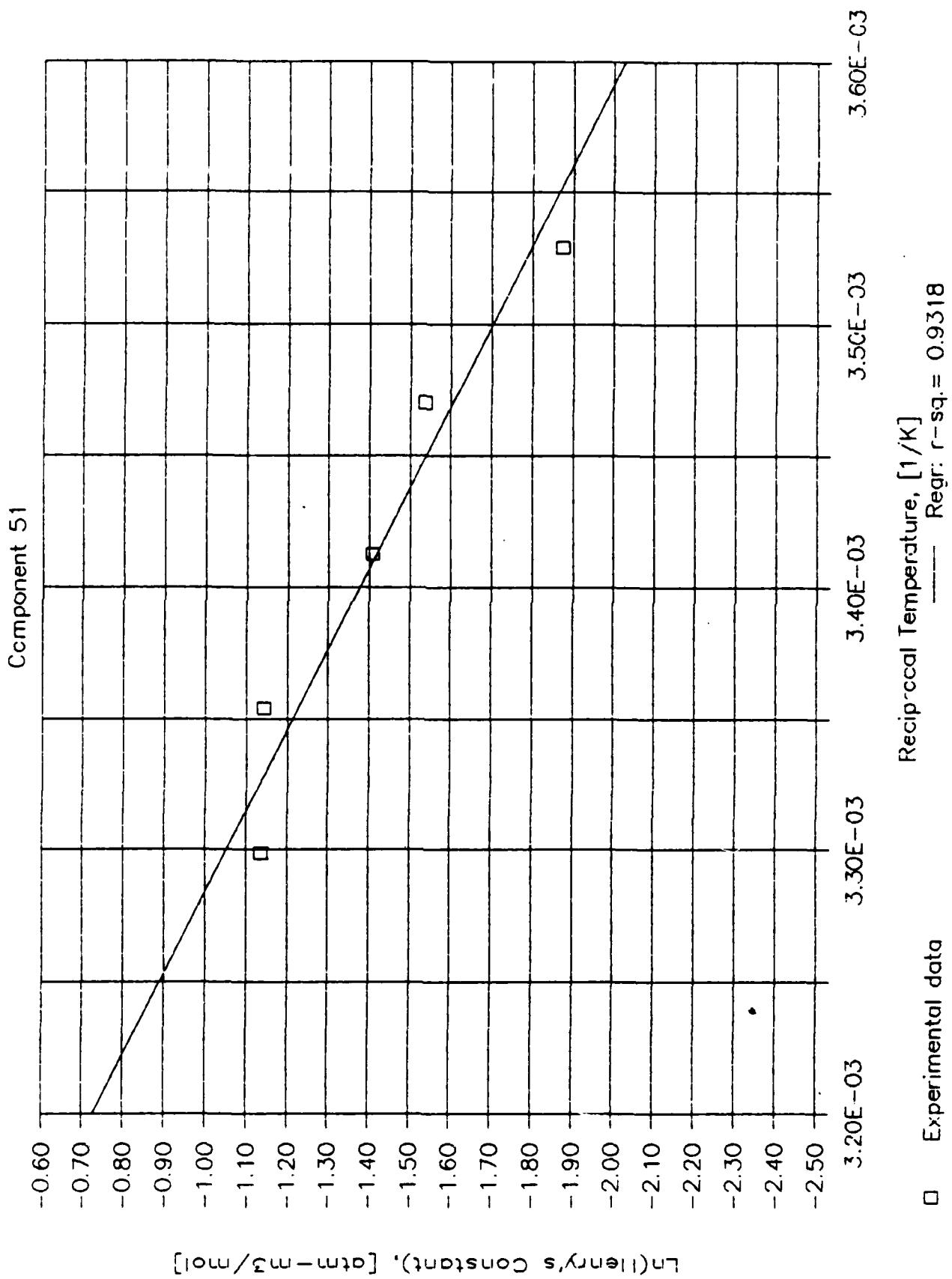
OF POINTS = 5

SLOPE = -3.2E+03

Y-INTERCEPT = 9.6E+00

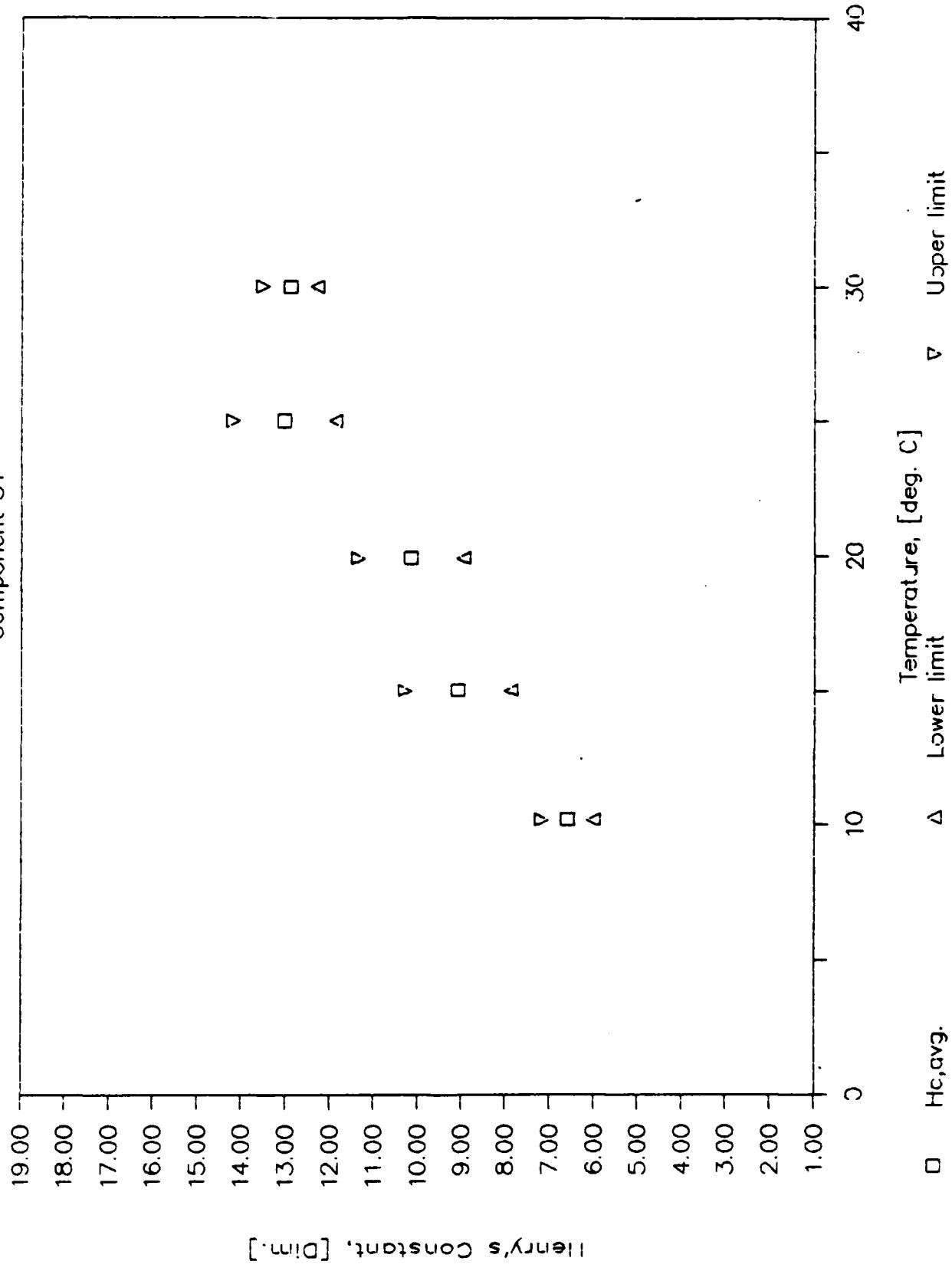
R-SQUARED = 0.9318

TEMPERATURE REGRESSION PLOT



95% CONFIDENCE TEST
Component 51

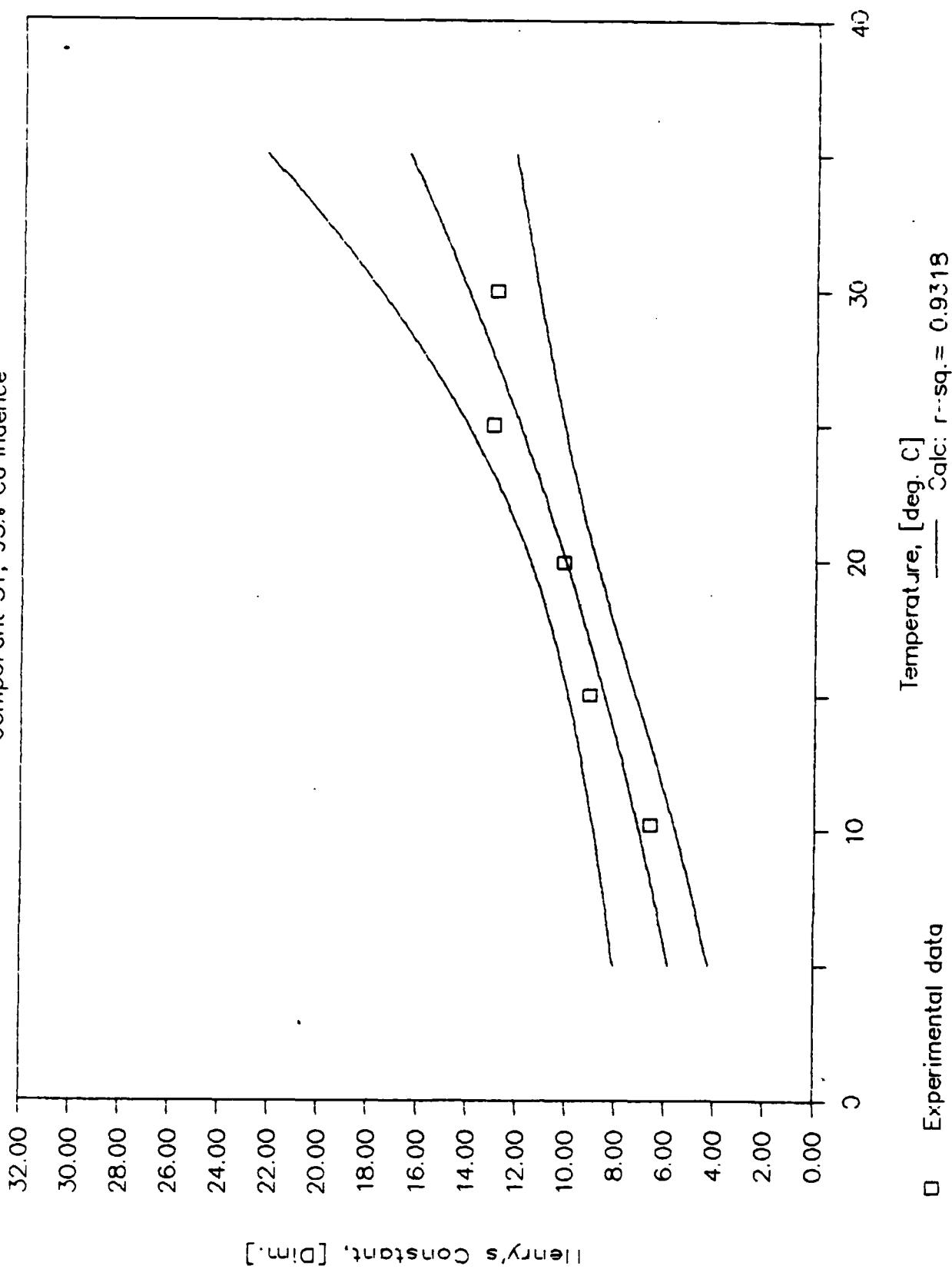
328



REGRESSION CONFIDENCE TEST

Component 51, 95% Confidence

329



04-Nov-86

Results Summary for Component 52

RUN Number	Temperature 1		Temperature 2		Temperature 3	
	1	13	13	25	25	25
REPLICATE	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	20		20		20	
Component ID	52		52		52	
Temperature (C)	10.1		15.1		19.6	
Low Vol (ml)	21		21		21	
High Vol (ml)	201		201		201	
System Vol (ml)	250		250		250	
H _{avg} : atm-m ³ /mol	0.0067	1.0E-25	0.0096	1.0E-25	0.0103	1.0E-25
H _{avg} : atm-mol/mol	8.7		12.6		13.7	
H _{avg} : atm-m ³ /mol	1.56E-04	1	2.27E-04	1	2.47E-04	1
H _{avg} : kPa-m ³ /mol	0.0158		0.0230		0.0250	
COV, r [std/mean]	119.86		41.57		27.74	
COV, both replic.	—		—		—	
Observation: (1)	-0.0001		0.0140		0.0113	
[atm-m ³ /mol] (2)	-0.0004		0.0073		0.0070	
(3)	0.0138		0.0118		0.0136	
(4)	0.0136		0.0053		0.0092	
Injection: (1)	27861		41436		53756	
[Peak Area] (2)	32000		40597		54941	
(3)	267080		345340		459360	
(4)	267710		367900		479000	

04-Nov-86

Results Summary (continued)

RUN Number -->	Temperature 4		Temperature 5	
	14	2	No. 1	No. 2
REPLICATE -->				
Group No.	20		20	
Component ID	52		52	
Temperature (C)	25		30	
Low Vol (ml)	21		21	
High Vol (ml)	201		201	
System Vol (ml)	250		250	
H, avg: atm-m3/m3	0.0100	1.0E-25	0.0118	1.0E-25
H, avg: atm-mol/mol	13.6		16.3	
H, avg: atm-m3/mol	2.45E-04	1	2.93E-04	1
H, avg: kPa-m3/mol	0.0248		0.0297	
COV, r [std/mean]	1.12		32.58	
COV, both replic.	_____		_____	
Observation: (1)	0.0101		0.0126	
(atm-m3/m3) (2)	0.0099		0.0165	
(3)	0.0101		0.0072	
(4)	0.0099		0.0109	
Injection: (1)	75644		107330	
[Peak Area] (2)	75648		101930	
(3)	653760		906060	
(4)	654980		874460	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

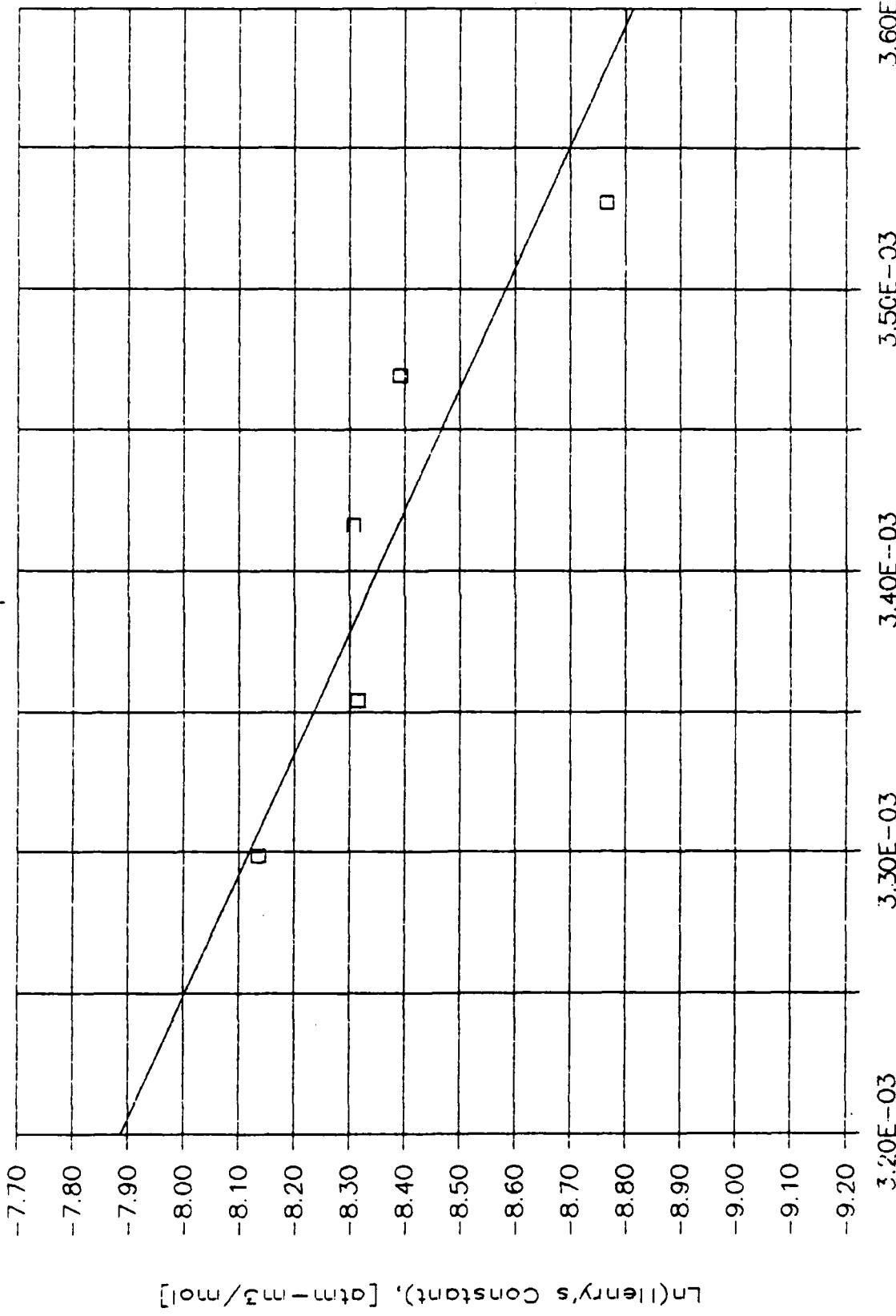
SLOPE = -2.3E+03

Y-INTERCEPT = -4.8E-01

R-SQUARED = 0.8229

TEMPERATURE REGRESSION PLOT

Component 52



□ Experimental data

Reciprocal Temperature, $[1/\text{K}]$

Regr: $r-\text{sq.} = 0.8229$

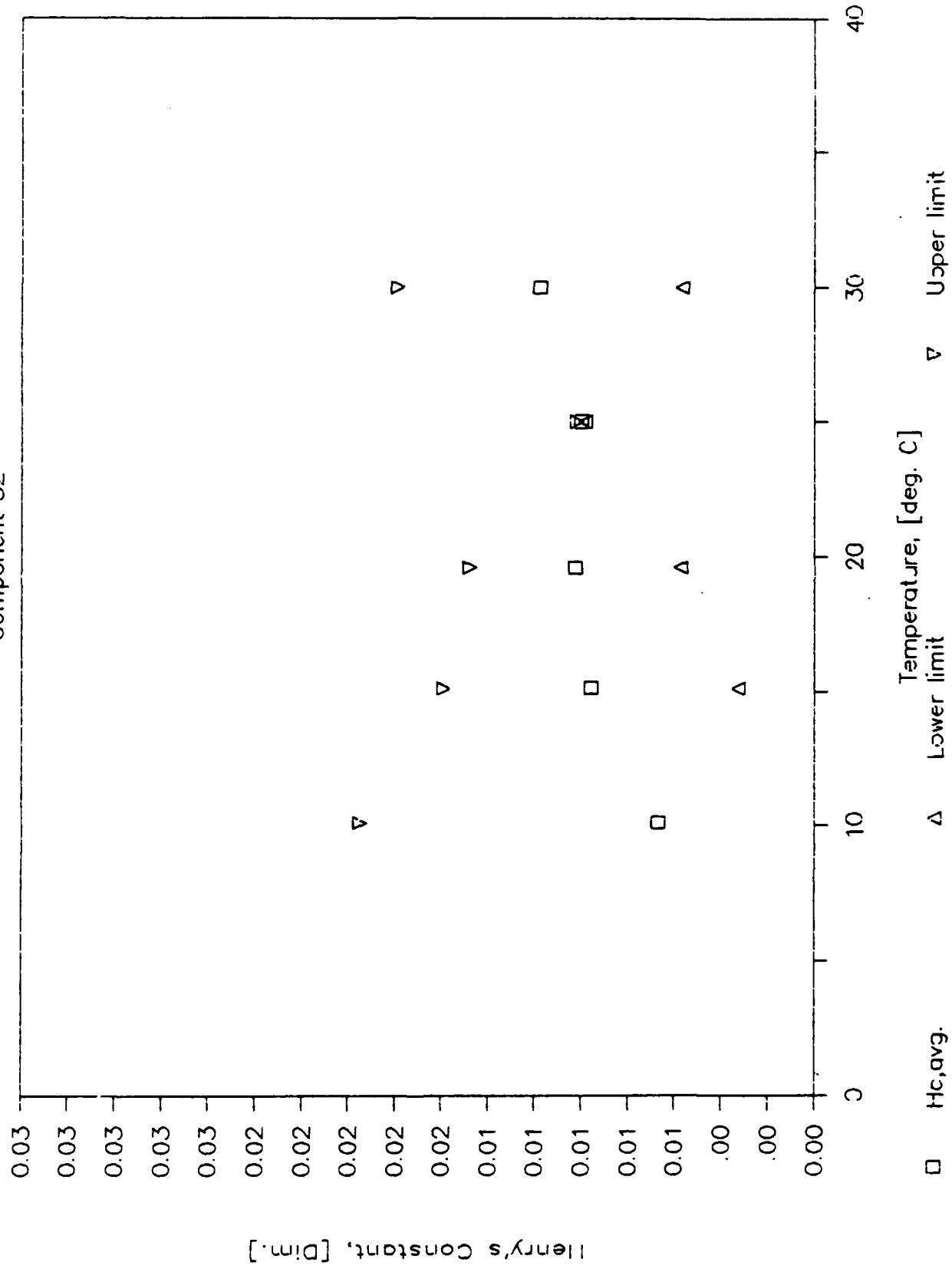
3.60E-03

3.50E-03

3.40E-03

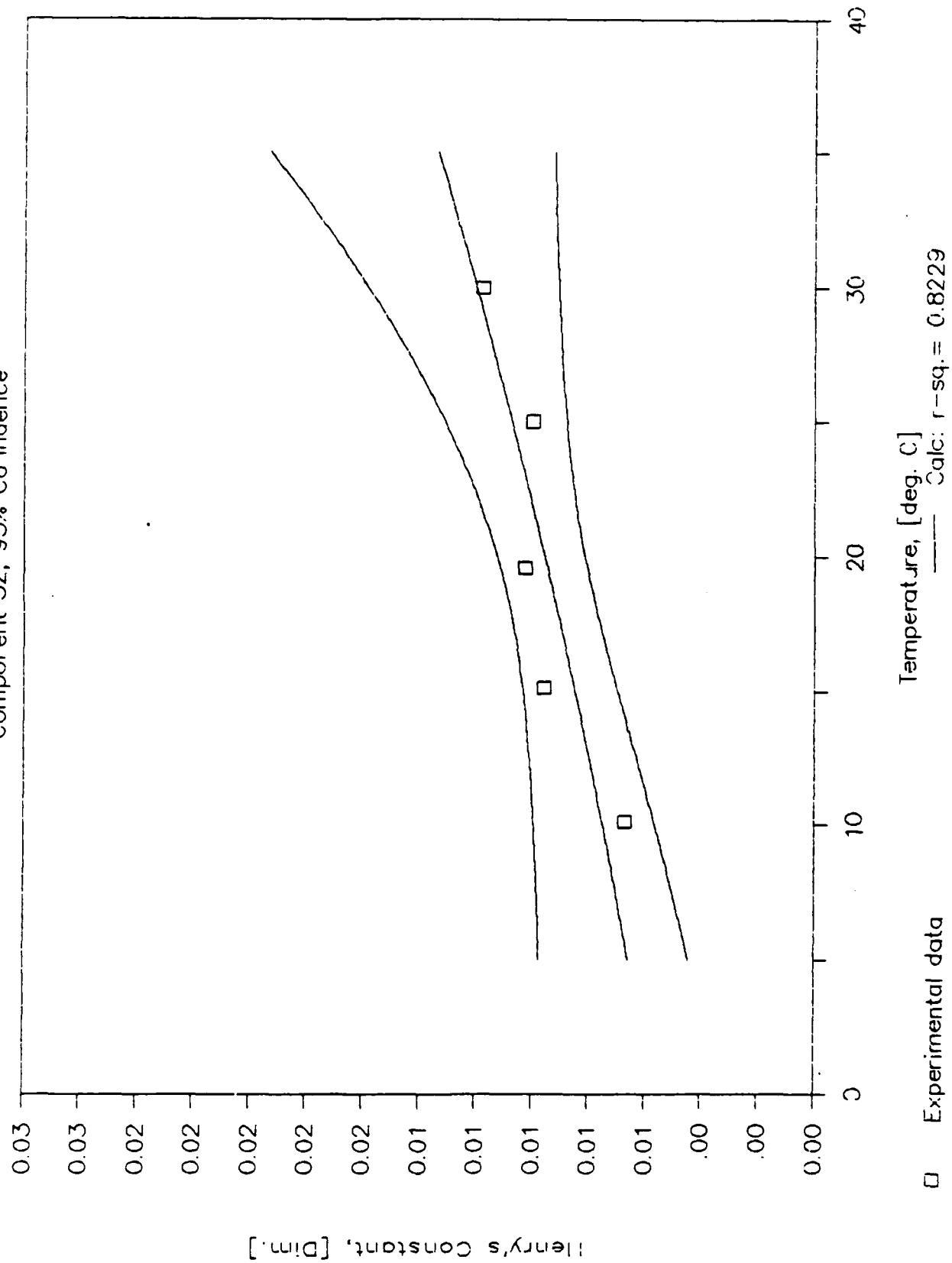
3.30E-03

95% CONFIDENCE TEST
Component 52



REGRESSION CONFIDENCE TEST

Component 52, 95% Confidence



12-Sep-86

Results Summary for Component 152

RUN Number →	Temperature 1		Temperature 2		Temperature 3	
	2	No. 1 No. 2	17	No. 1 No. 2	52	No. 1 No. 2
REPLICATE →						
Group No.	20		20		20	
Component ID	152		152		152	
Temperature (C)	10.5		15.1		20.2	
Low Vol (ml)	21		21		21	
High Vol (ml)	201		201		201	
System Vol (ml)	250		250		250	
H _a avg: atm-m ³ /m ³	0.0120	1.0E-25	0.0166	1.0E-25	0.0077	1.0E-25
H _a avg: atm-mol/mol	15.5		21.8		10.3	
H _a avg: atm-m ³ /mol	2.79E-04	1	3.92E-04	1	1.85E-04	1
H _a avg: kPa-m ³ /mol	0.0282		0.0397		0.0188	
COV, r [std/mean]	35.50		21.40		6.32	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0161		0.0143		0.0080	
[atm-m ³ /m ³] (2)	0.0151		0.0129		0.0072	
(3)	0.0088		0.0203		0.0082	
(4)	0.0078		0.0188		0.0074	
Injection: (1)	33042		43700		49633	
[Peak Area] (2)	30852		46110		49719	
(3)	269990		363080		437630	
(4)	272570		367890		441190	

12-Sep-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		17		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		20		20	
Component ID		152		152	
Temperature (C)		25.2		30	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H _v avg: atm-m ³ /m ³		0.0053	1.0E-25	0.0044	1.0E-25
H _v avg: atm-mol/mol		7.2		6.1	
H _v avg: atm-m ³ /mol		1.30E-04	1	1.10E-04	1
H _v avg: kPa-m ³ /mol		0.0131		0.0112	
COV, r [std/mean]		81.79		19.78	
COV, both replic.		_____		_____	
Observation: (1)		0.0098		0.0055	
[atm-m ³ /m ³] (2)		0.0082		0.0047	
(3)		0.0024		0.0041	
(4)		0.0009		0.0034	
Injection: (1)		78786		100440	
[Peak Area] (2)		73177		99088	
(3)		683190		908580	
(4)		693890		915260	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

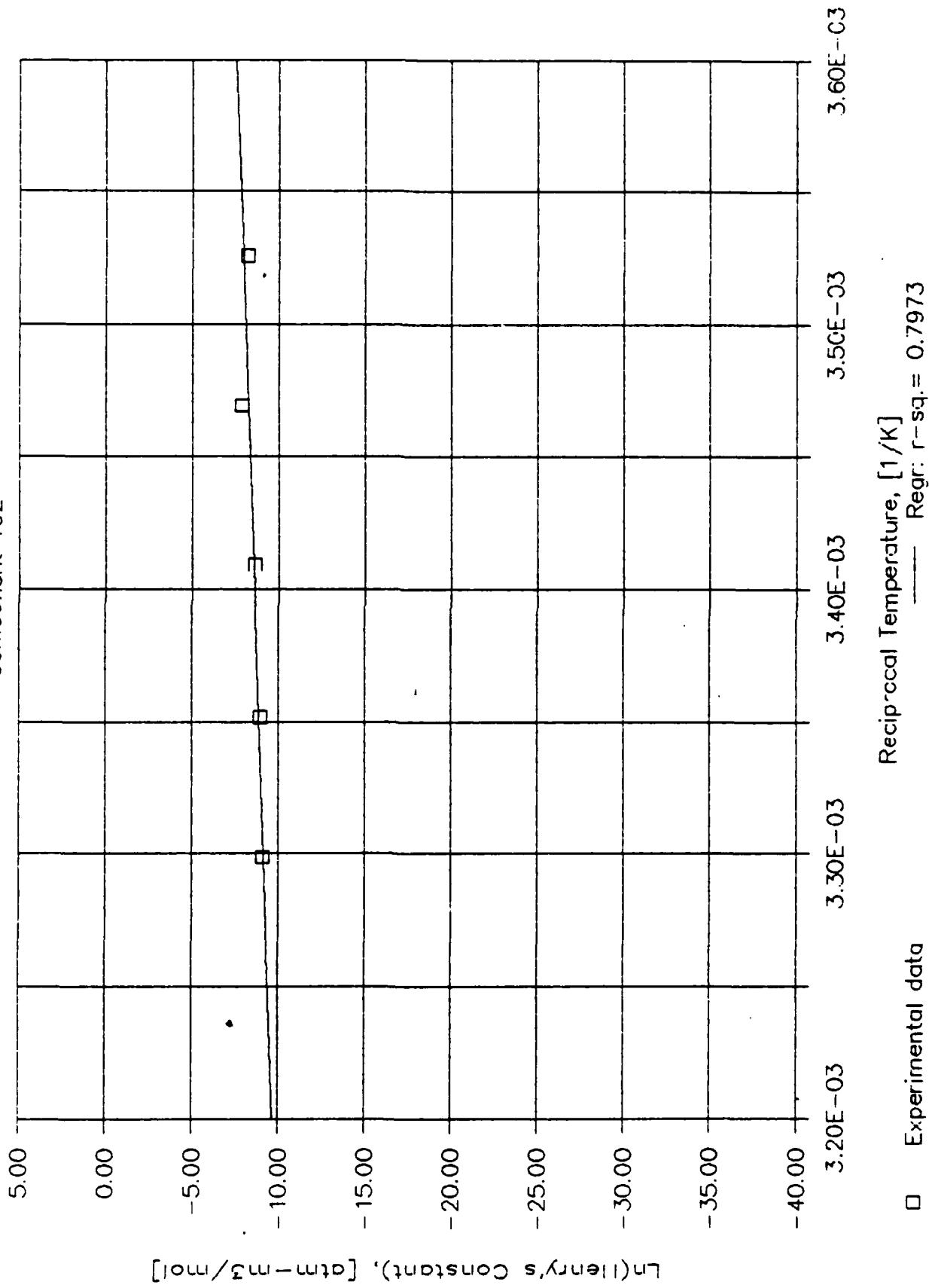
SLOPE = 5.2E+03

Y-INTERCEPT = -2.6E+01

R-SQUARED = 0.7973

TEMPERATURE REGRESSION PLOT

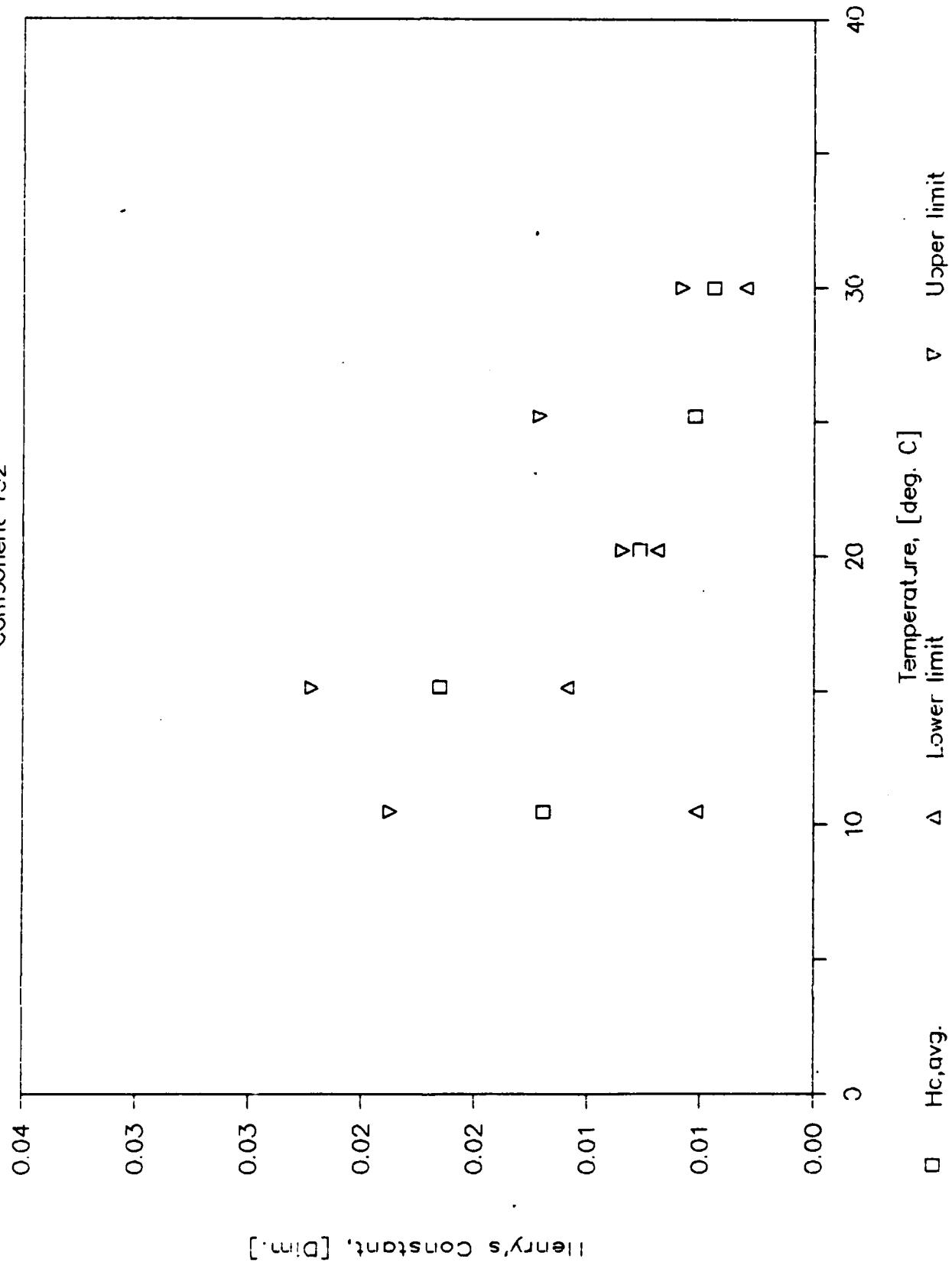
Component 15.2



95% CONFIDENCE TEST

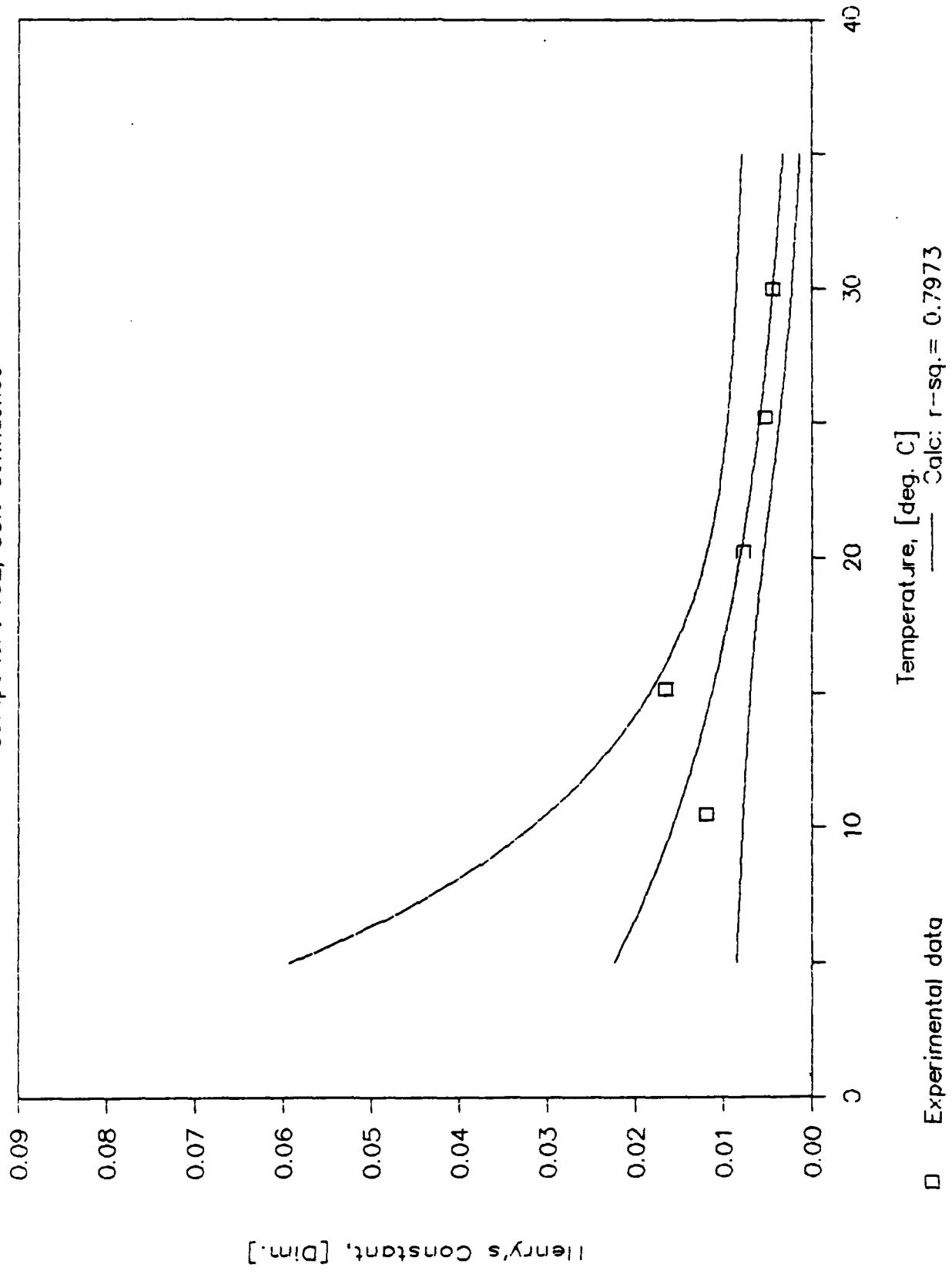
Component 152

338



REGRESSION CONFIDENCE TEST

Component 152, 95% Confidence



04-Nov-86

Results Summary for Component 53

RUN Number -->	Temperature 1		Temperature 2		Temperature 3	
	5		17		28	
REPLICATE -->	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.	20		20		20	
Component ID	53		53		53	
Temperature (C)	10.1		15.1		19.6	
Low Vol (ml)	21		21		21	
High Vol (ml)	201		201		201	
System Vol (ml)	250		250		250	
H _a avg: atm-m ³ /mol	0.0283	1.0E-25	0.0157	1.0E-25	0.0119	1.0E-25
H _a avg: atm-mol/mol	36.6		20.7		15.9	
H _a avg: atm-m ³ /mol	6.59E-04	1	3.72E-04	1	2.87E-04	1
H _a avg: kPa-m ³ /mol	0.0667		0.0377		0.0291	
COV, r [std/mean]	28.47		2.80		35.36	
COV, both replic.	_____		_____		_____	
Observation: (1)	0.0332		0.0162		0.0112	
[atm-m ³ /mol] (2)	0.0370		0.0155		0.0171	
(3)	0.0199		0.0160		0.0069	
(4)	0.0232		0.0153		0.0125	
Injection: (1)	59140		70407		105580	
[Peak Area] (2)	53007		70262		101240	
(3)	418840		574850		902890	
(4)	407100		578660		854970	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		18		6	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		20		20	
Component ID		53		53	
Temperature (C)		25		30	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H ₄ avg: atm-m ³ /mol		0.0159	1.0E-25	0.0272	1.0E-25
H ₄ avg: atm-mol/mol		21.6		37.6	
H ₄ avg: atm-m ³ /mol		3.89E-04	1	6.78E-04	1
H ₄ avg: kPa-m ³ /mol		0.0394		0.0687	
COV, r [std/mean]		36.14		11.55	
COV, both replic.		_____		_____	
Observation: (1)		0.0174		0.0237	
[atm-m ³ /mol]	(2)	0.0092		0.0287	
	(3)	0.0229		0.0257	
	(4)	0.0142		0.0308	
Injection:	(1)	128050		200340	
[Peak Area]	(2)	134300		203720	
	(3)	1034700		1532400	
	(4)	1116900		1470500	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

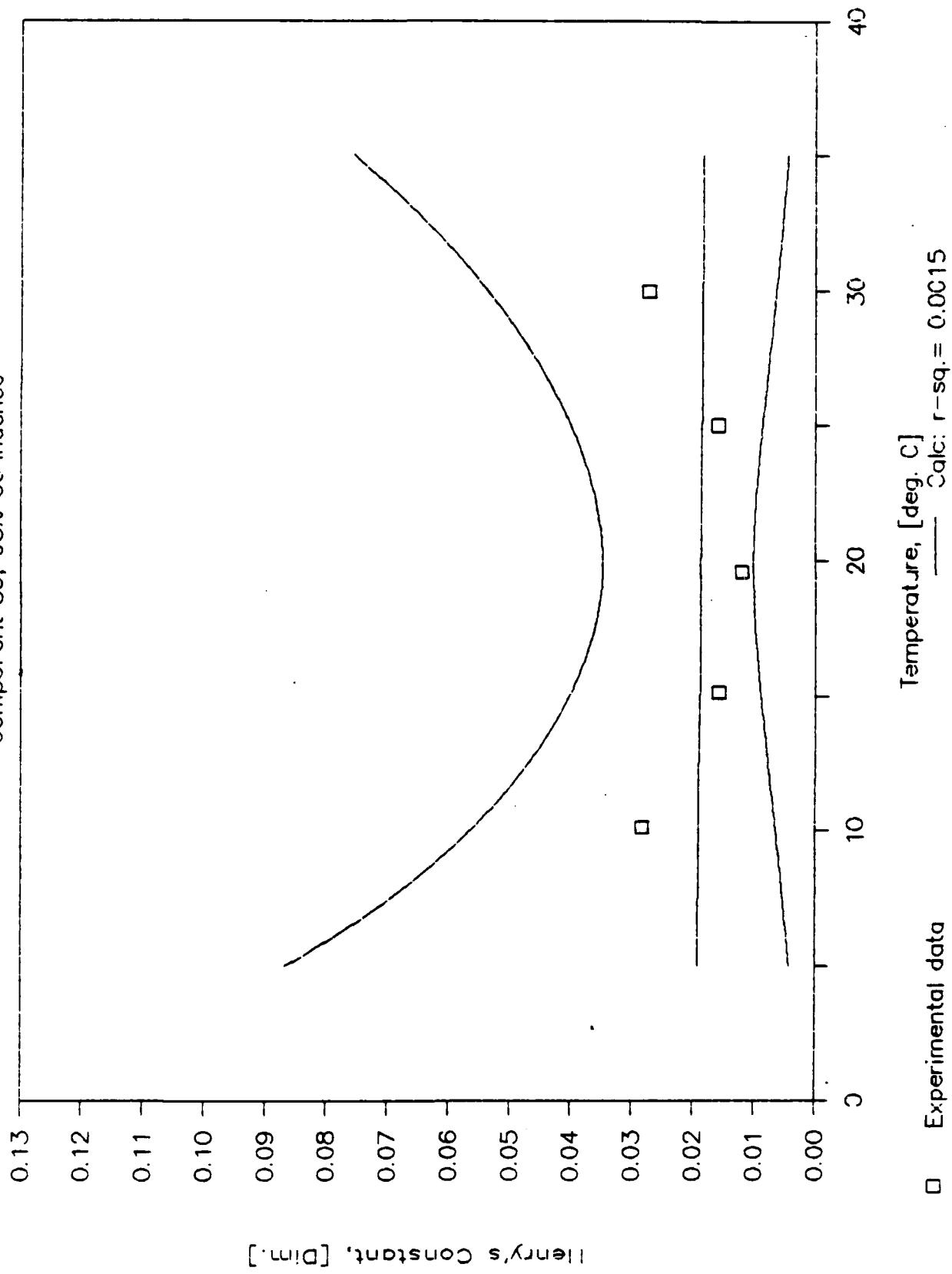
SLOPE = -1.6E+02

Y-INTERCEPT = -7.2E+00

R-SQUARED = 0.0015

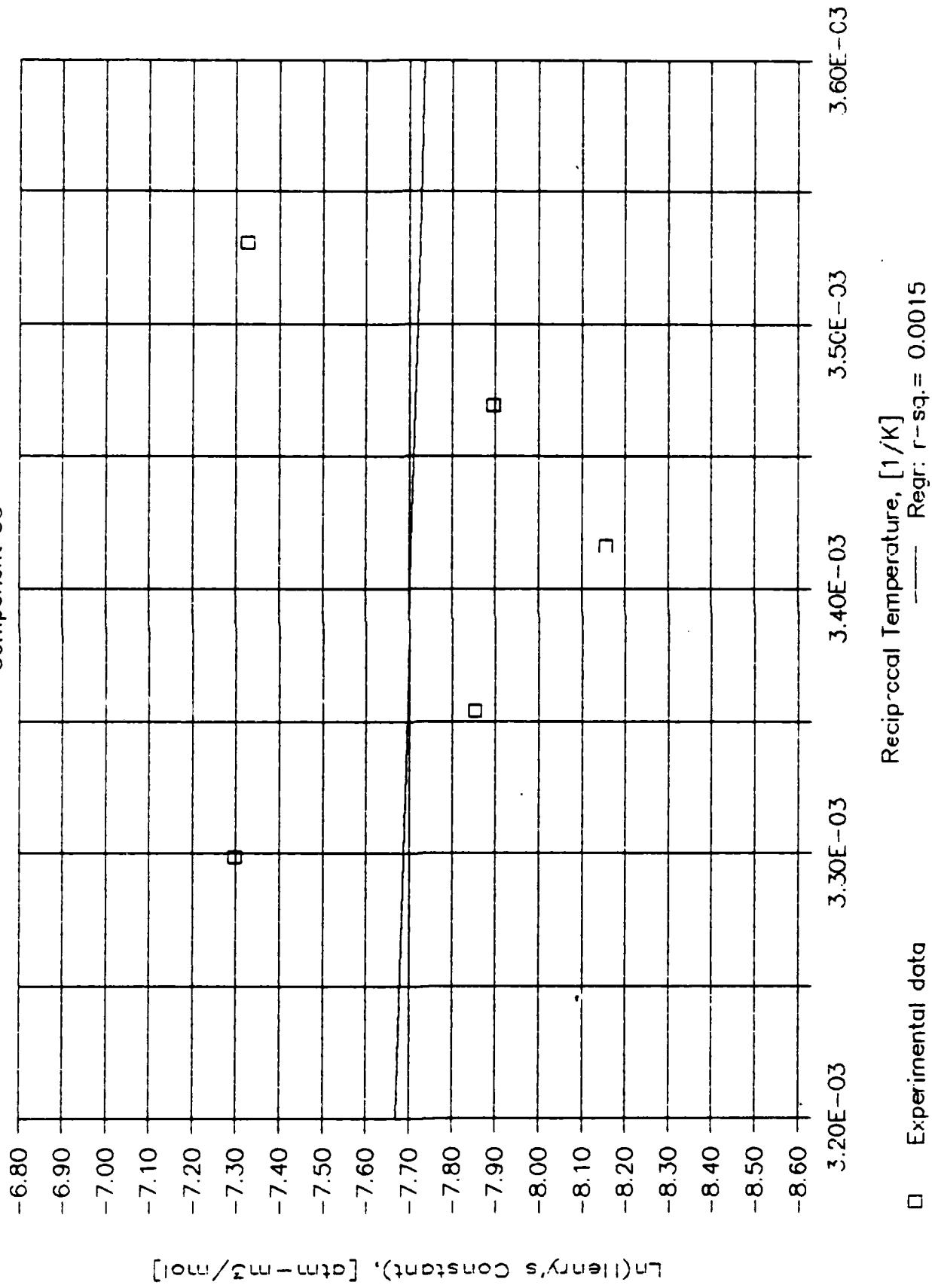
REGRESSION CONFIDENCE TEST

Component 53, 95% Confidence



TEMPERATURE REGRESSION PLOT

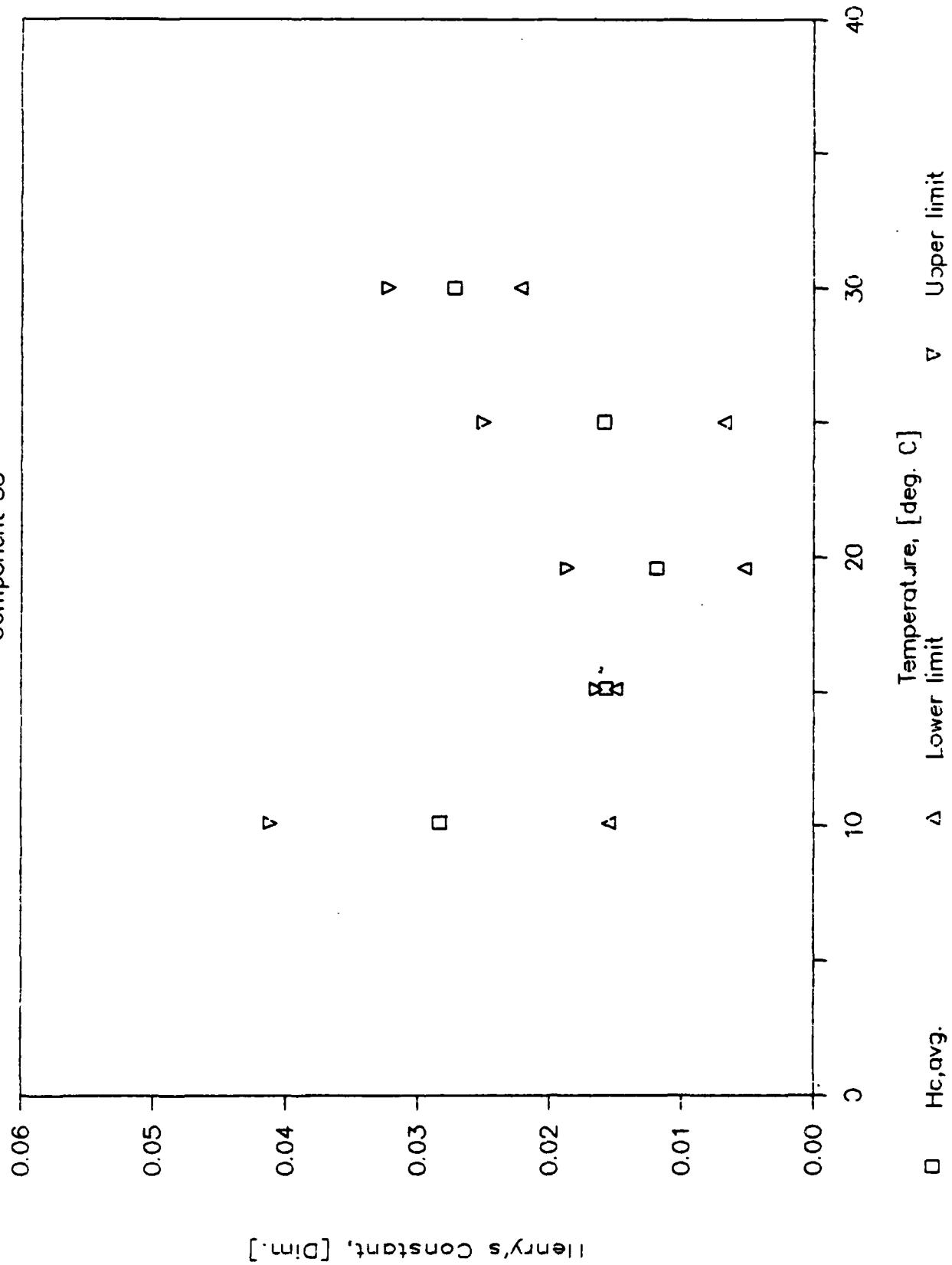
Component 53



95% CONFIDENCE TEST

Component 53

344



12-Sep-86

Results Summary for Component 153

RUN Number —>	Temperature 1		Temperature 2		Temperature 3	
	7	No. 1	No. 2	24	No. 1	No. 2
REPLICATE —>						
Group No.	20			20		20
Component ID	153			153		153
Temperature (C)	10.5			15.1		20.1
Low Vol (ml)	21			21		21
High Vol (ml)	201			201		201
System Vol (ml)	250			250		250
H ₄ avg: atm-m ³ /m ³	0.0053	1.0E-25		0.0048	1.0E-25	
H ₄ avg: mol/mol	6.8			6.3		5.8
H ₄ avg: atm-m ³ /mol	1.23E-04	1		1.14E-04	1	1.04E-04
H ₄ avg: kPa-m ³ /mol	0.0125			0.0116		0.0105
COV, r [std/mean]	60.64			18.25		18.49
COV, both replic.	_____			_____		_____
Observation: (1)	0.0076			0.0047		0.0048
[atm-m ³ /m ³] (2)	0.0085			0.0038		0.0035
(3)	0.0021			0.0059		0.0052
(4)	0.0030			0.0050		0.0039
Injection: (1)	83452			111840		161020
[Peak Area] (2)	78971			113230		161670
(3)	739210			1019700		1466500
(4)	732630			1029200		1486400

12-Sep-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		25		8	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		20		20	
Component ID		153		153	
Temperature (C)		25.2		30	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H, avg: atm-m3/mol		0.0079 1.0E-25		0.0063 1.0E-25	
H, avg: atm-mol/mol		10.7		8.7	
H, avg: atm-m3/mol		1.93E-04	1	1.57E-04	1
H, avg: kPa-m3/mol		0.0196		0.0159	
COV, r [std/mean]		19.09		28.96	
COV, both replic.		_____		_____	
Observation: (1)		0.0085		0.0080	
[atm-m3/mol] (2)		0.0062		0.0077	
(3)		0.0096		0.0049	
(4)		0.0073		0.0046	
Injection: (1)		231040		319490	
[Peak Area] (2)		233660		309630	
(3)		2028300		2816900	
(4)		2075400		2825900	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

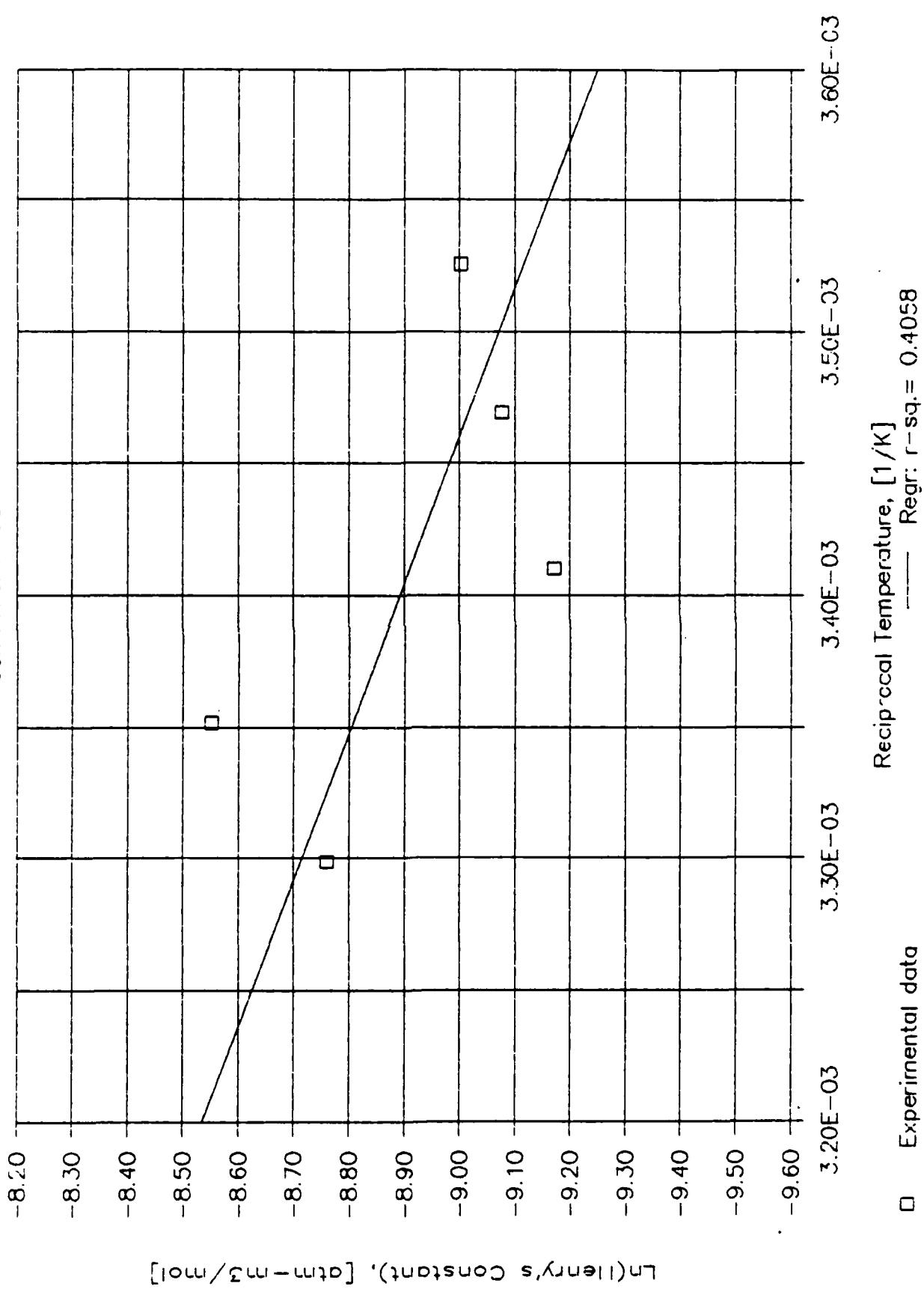
SLOPE = -1.8E+03

Y-INTERCEPT = -2.8E+00

R-SQUARED = 0.4058

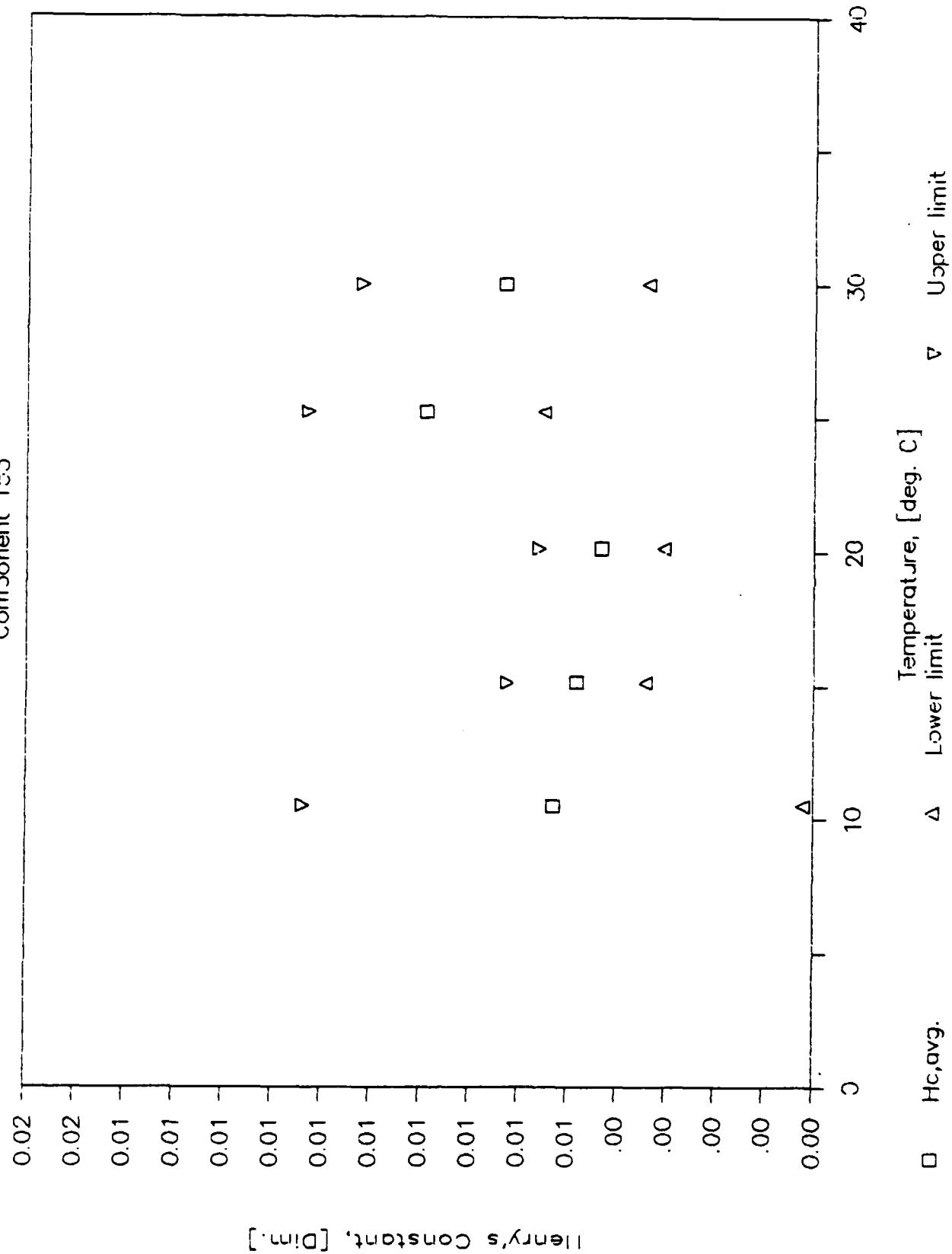
TEMPERATURE REGRESSION PLOT

Component 15.3



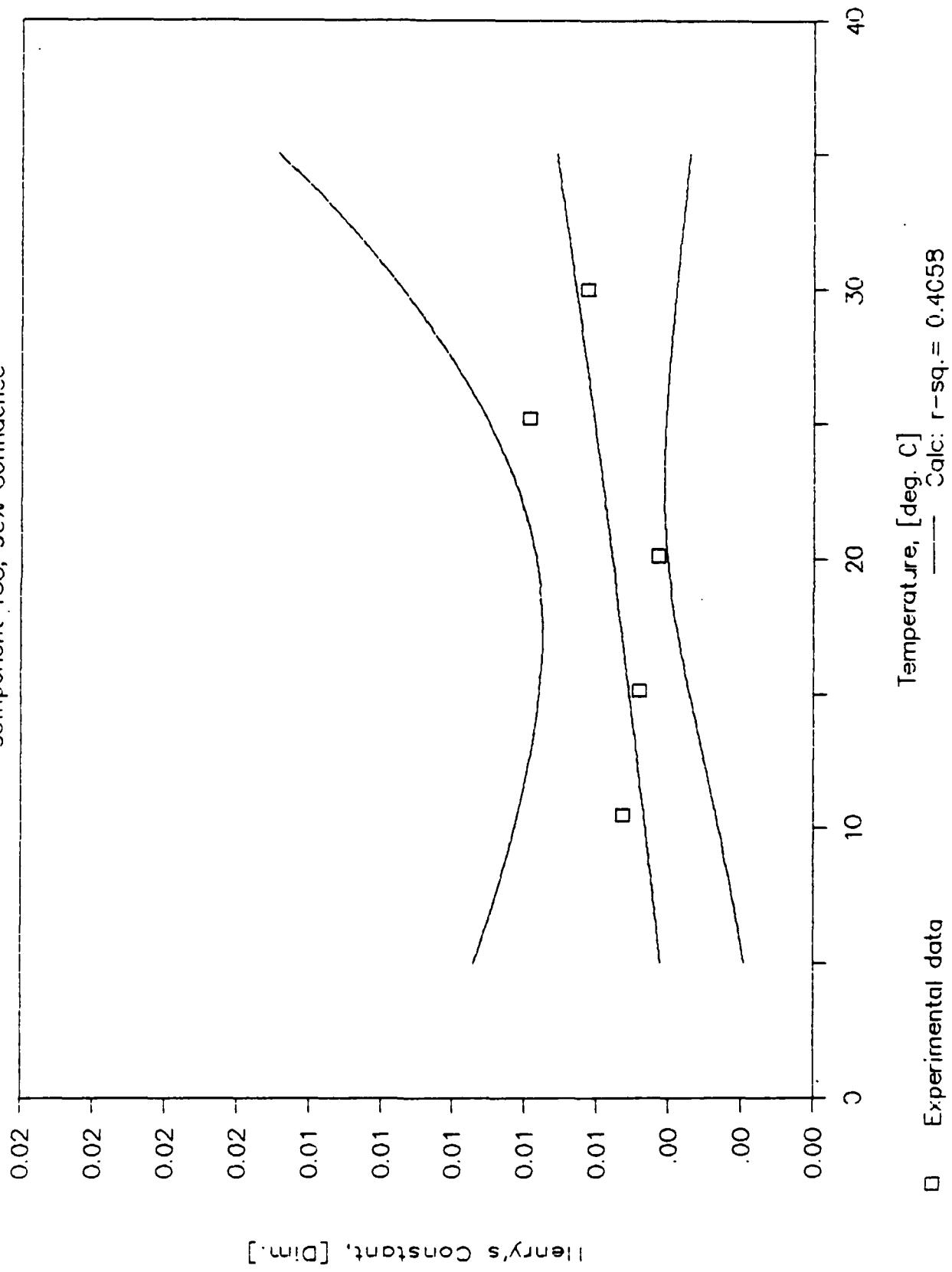
95% CONFIDENCE TEST

348



REGRESSION CONFIDENCE TEST

Component 153, 95% Confidence



04-Nov-86

Results Summary for Component 54

		Temperature 1		Temperature 2		Temperature 3	
RUN Number -->		9	-	21	-	33	-
REPLICATE -->		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		20		20		20	
Component ID		54		54		54	
Temperature (C)		10.1		15.1		19.6	
Low Vol (ml)		21		21		21	
High Vol (ml)		201		201		201	
System Vol (ml)		250		250		250	
H ₄ avg: atm-m ³ /m ³		1.8980	1.0E-25	1.5346	1.0E-25	4.8118	1.0E-25
H ₄ avg: atm-mol/mol		2448.7		2014.9		6416.2	
H ₄ avg: atm-m ³ /mol		4.41E-02	1	3.63E-02	1	1.16E-01	1
H ₄ avg: kPa-m ³ /mol		4.4700		3.6781		11.7125	
COV, r [std/mean]		33.20		16.07		32.33	
COV, both replic.		_____		_____		_____	
Observation: (1)		2.3451		1.8051		6.7888	
[atm-m ³ /m ³] (2)		2.5324		1.6763		5.2461	
(3)		1.3124		1.3750		3.9636	
(4)		1.4019		1.2822		3.2486	
Injection: (1)		55588		22968		49104	
[Peak Area] (2)		38139		19154		39079	
(3)		31469		15305		16631	
(4)		30072		16062		18401	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		22		10	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		20		20	
Component ID		54		54	
Temperature (C)		25		30	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H,avg: atm-m3/mol		1.2640	1.0E-25	1.5326	1.0E-25
H,avg: atm-mol/mol		1716.6		2116.2	
H,avg: atm-m3/mol		3.09E-02	1	3.81E-02	1
H,avg: kPa-m3/mol		3.1336		3.8631	
COV, r [std/mean]		16.03		15.85	
COV, both replic.		_____		_____	
Observation: (1)		1.5094		1.8225	
[atm-m3/m3] (2)		1.1723		1.6266	
(3)		1.3335		1.4128	
(4)		1.0409		1.2685	
Injection: (1)		21149		48750	
[Peak Area] (2)		19435		41163	
(3)		15860		32285	
(4)		18883		34777	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

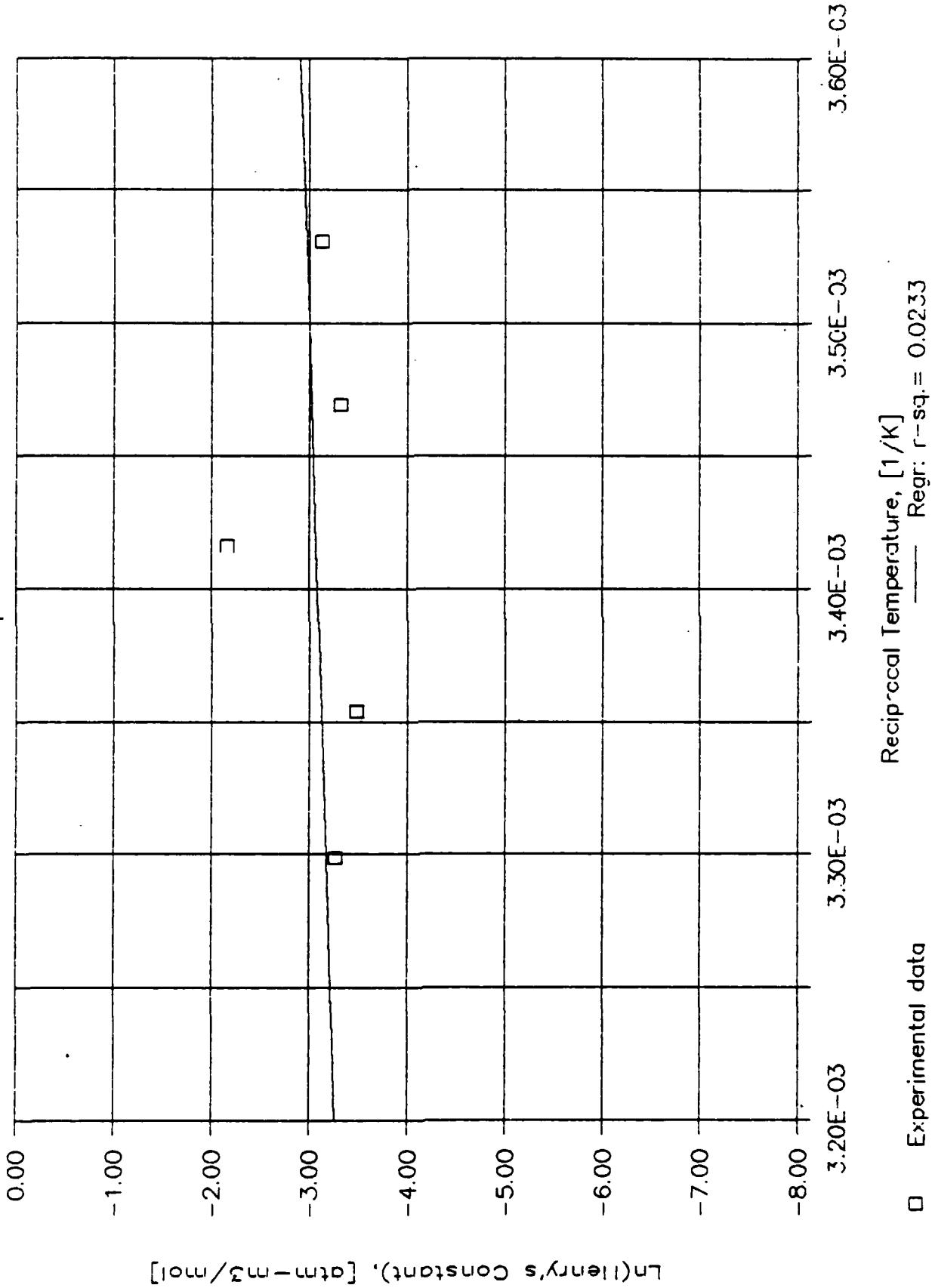
SLOPE = 8.7E+02

Y-INTERCEPT = -6.1E+00

R-SQUARED = 0.0233

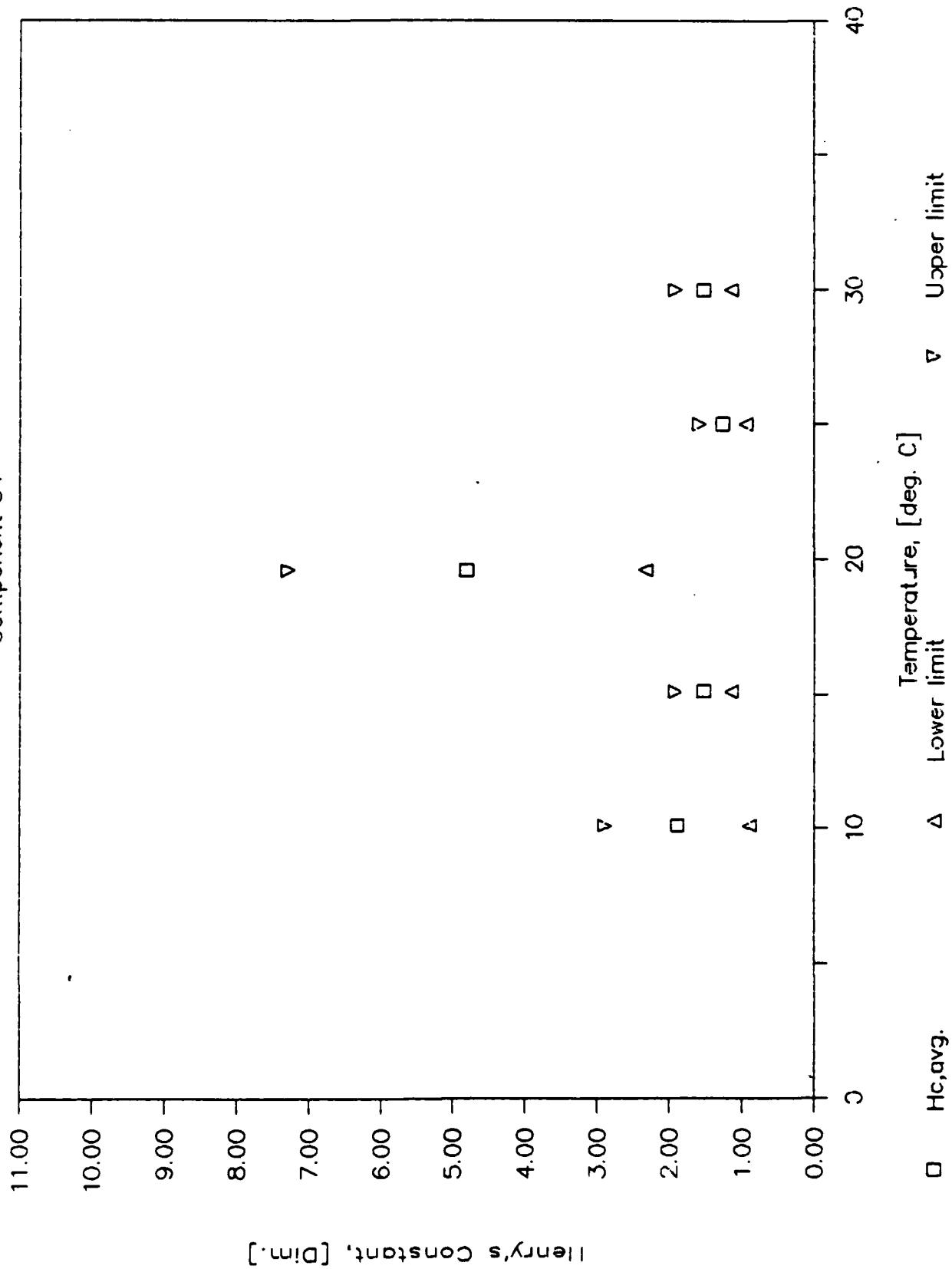
TEMPERATURE REGRESSION PLOT

Component 54



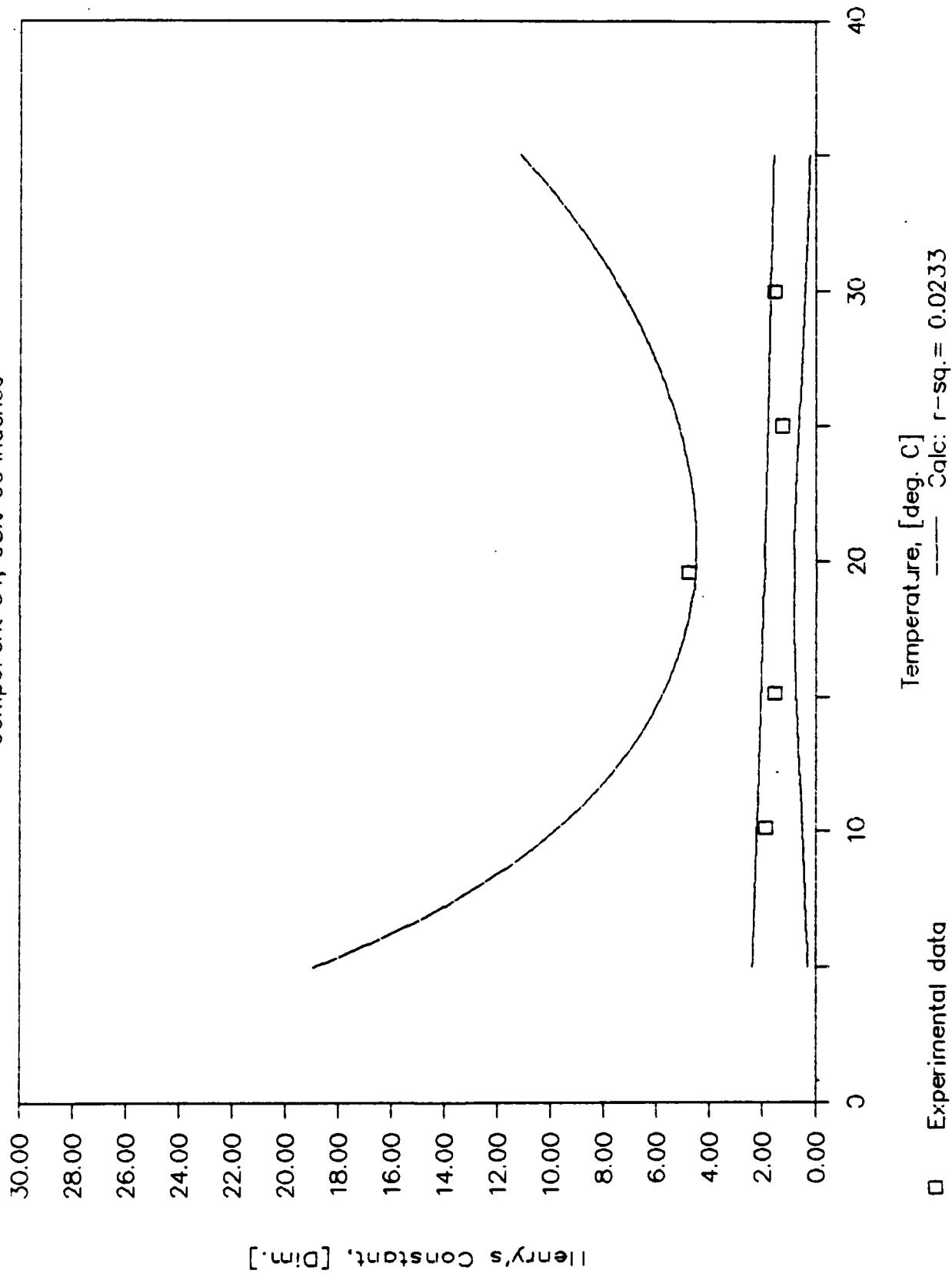
95% CONFIDENCE TEST

Component 54



REGRESSION CONFIDENCE TEST

Component 54, 95% Confidence



04-Nov-86

Results Summary for Component 55

		Temperature 1		Temperature 2		Temperature 3	
RUN-Number	→	2		10		2	
REPLICATE	→	No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		21		21		21	
Component ID		55		55		55	
Temperature (C)		10.1		15.1		20.2	
Low Vol (ml)		21		21		21	
High Vol (ml)		201		201		201	
System Vol (ml)		250		250		250	
H _c avg: atm-m ³ /m ³		0.0537	1.0E-25	0.0067	1.0E-25	0.0299	1.0E-25
H _c avg: atm-mol/mol		69.2		8.8		40.0	
H _c avg: atm-m ³ /mol		1.25E-03	1	1.58E-04	1	7.20E-04	1
H _c avg: kPa-m ³ /mol		0.1264		0.0160		0.0730	
COV, r [std/mean]		75.96		347.46		28.41	
COV, both replic.		_____		_____		_____	
Observation: (1)		0.0770		0.0293		0.0247	
[atm-m ³ /m ³] (2)		0.0986		0.0242		0.0209	
(3)		0.0129		-0.0117		0.0391	
(4)		0.0261		-0.0150		0.0349	
Injection: (1)		4672		4779		6407	
[Peak Area] (2)		2943		3194		7174	
(3)		24768		34922		48590	
(4)		22065		36418		50179	

04-Nov-86

Results Summary (continued)

		Temperature 4		Temperature 5	
RUN Number -->		11		3	
REPLICATE -->		No. 1	No. 2	No. 1	No. 2
Group No.		21		21	
Component ID		55		55	
Temperature (C)		25.2		30	
Low Vol (ml)		21		21	
High Vol (ml)		201		201	
System Vol (ml)		250		250	
H _a avg: atm-m ³ /m ³		0.0051	1.0E-25	0.0006	1.0E-25
H _a avg: atm-mol/mol		7.0		0.8	
H _a avg: atm-m ³ /mol		1.26E-04	1	1.38E-05	1
H _a avg: kPa-m ³ /mol		0.0127		0.0014	
COV, r [std/mean]		92.84		697.60	
COV, both replic.		_____		_____	
Observation: (1)		0.0108		0.0045	
[atm-m ³ /m ³] (2)		0.0034		-0.0021	
(3)		0.0067		0.0031	
(4)		-0.0004		-0.0034	
Injection: (1)		8564		10942	
[Peak Area] (2)		8230		10785	
(3)		73520		99903	
(4)		79100		107090	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

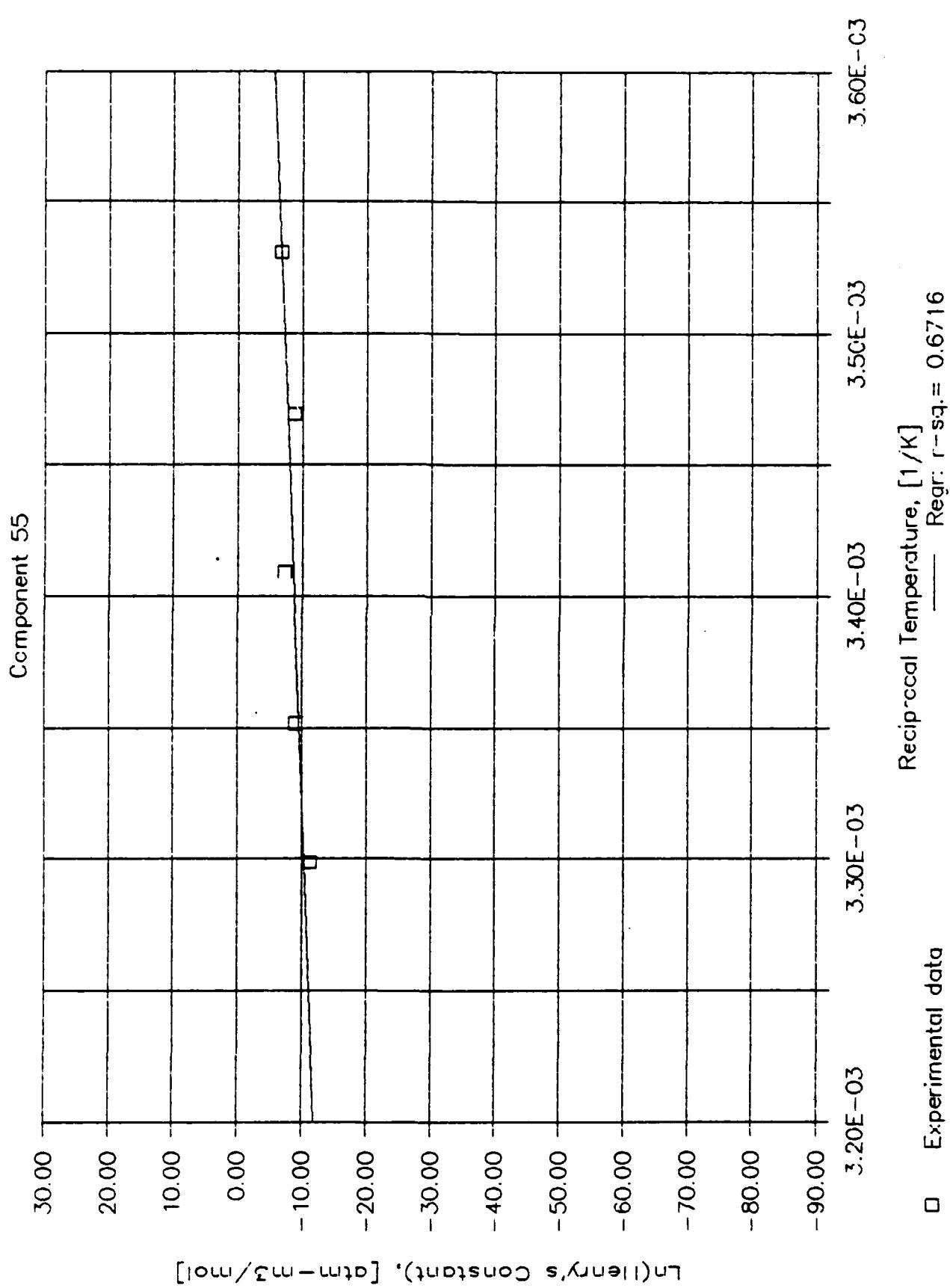
OF POINTS = 5

SLOPE = 1.6E+04

Y-INTERCEPT = -6.2E+01

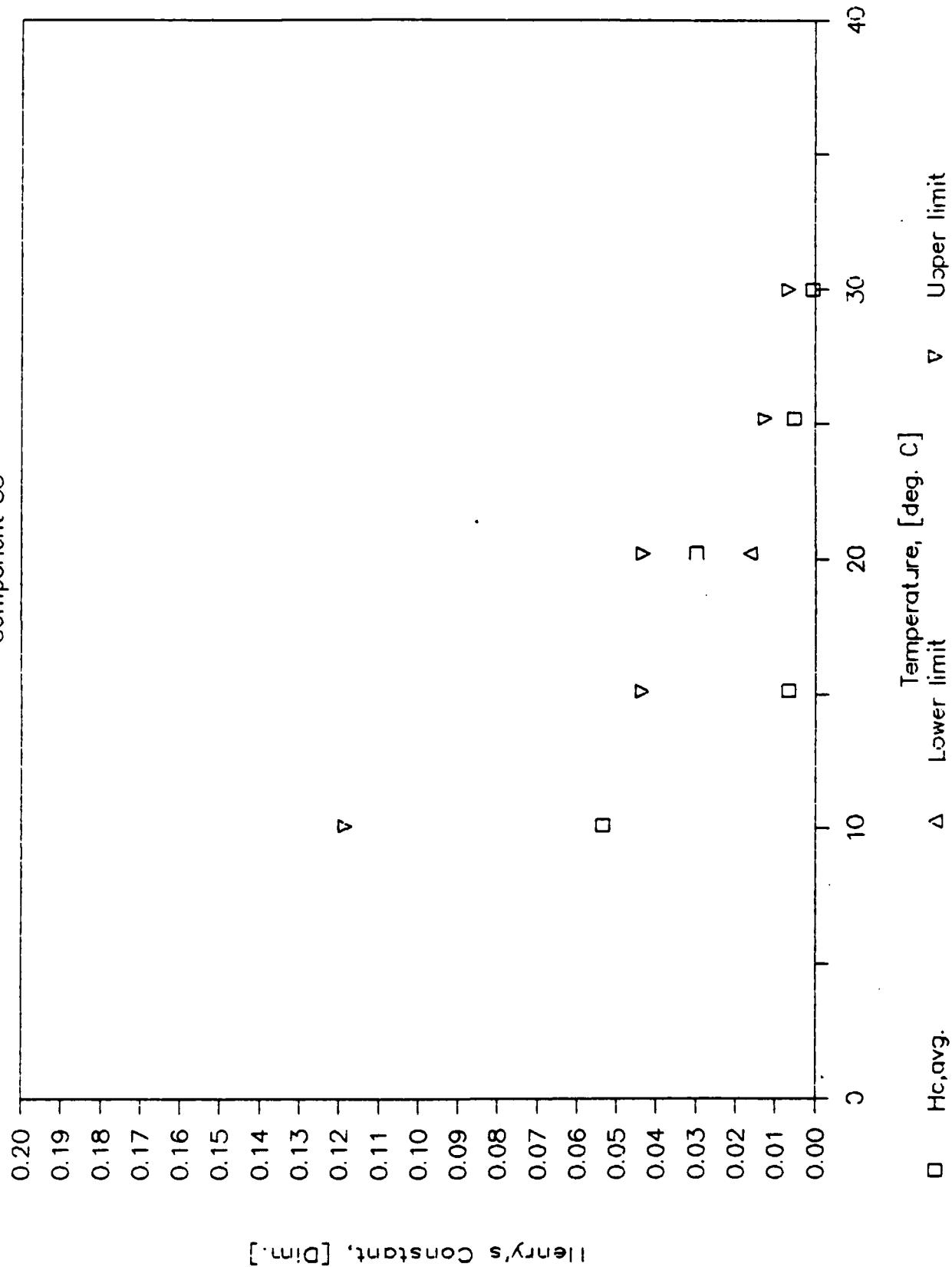
R-SQUARED = 0.6716

TEMPERATURE REGRESSION PLOT



95% CONFIDENCE TEST
Component 55

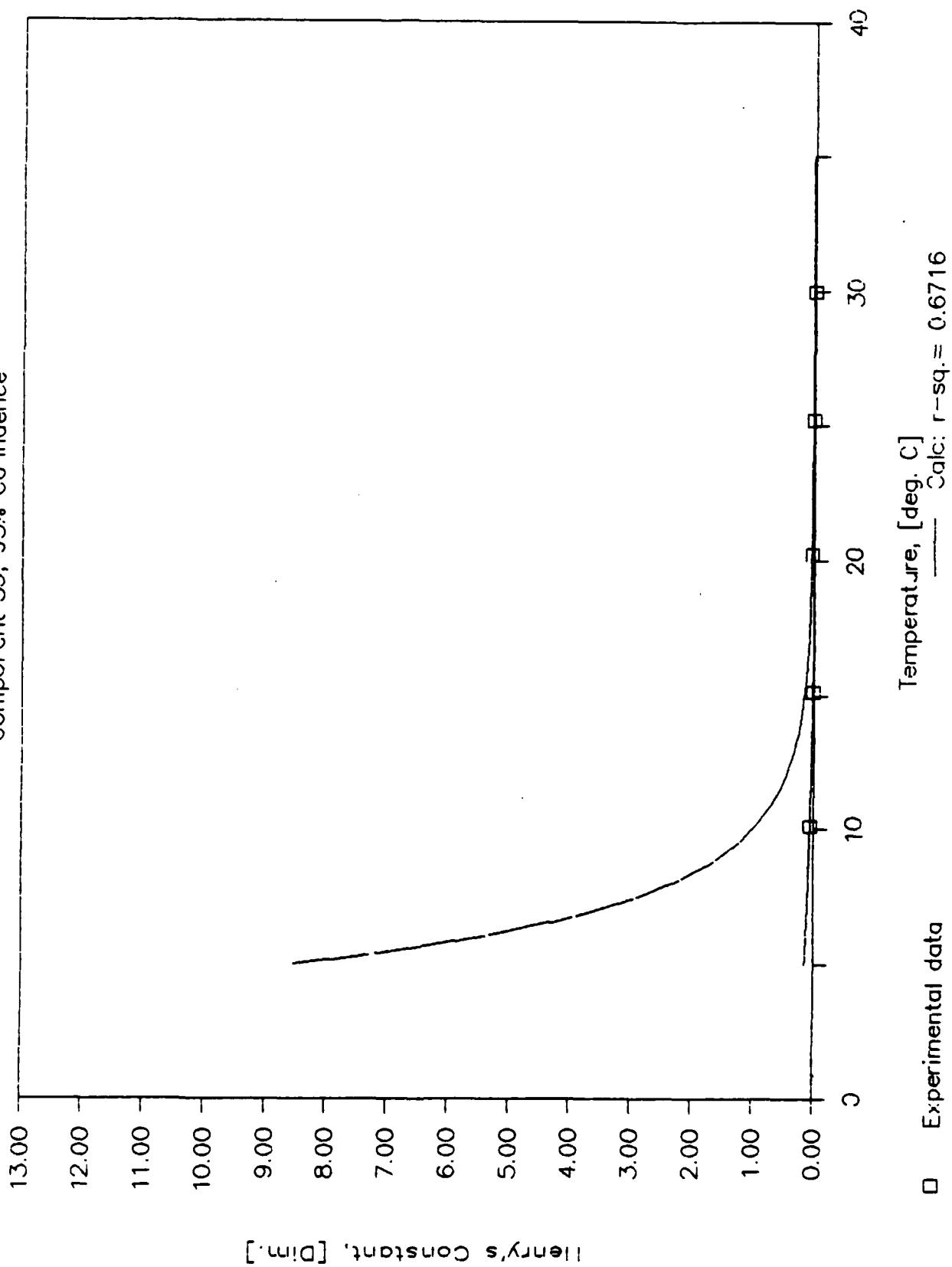
358



Henry's Constant, [Dim.]

REGRESSION CONFIDENCE TEST

Component 55, 95% Confidence



04-Nov-86

Results Summary for Component 56

		Temperature 1		Temperature 2		Temperature 3	
RUN Number →		6		13		5	
REPLICATE →		No. 1	No. 2	No. 1	No. 2	No. 1	No. 2
Group No.		21		21		21	
Component ID		56		56		56	
Temperature (C)		10.1		15.1		20.2	
Low Vol (ml)		21		21		21	
High Vol (ml)		201		201		201	
System Vol (ml)		250		250		250	
H, avg: atm-m3/mol		2.3040	1.0E-25	2.8738	1.0E-25	3.3397	1.0E-25
H, avg: atm-mol/mol		2972.5		3773.1		4462.3	
H, avg: atm-m3/mol		5.36E-02	1	6.80E-02	1	8.04E-02	1
H, avg: kPa-m3/mol		5.4263		6.8878		8.1459	
COV, r [std/mean]		6.47		0.57		1.07	
COV, both replic.		_____		_____		_____	
Observation: (1)		2.1279		2.8547		3.3816	
[atm-m3/mol] (2)		2.2743		2.8682		3.3523	
(3)		2.3245		2.8793		3.3267	
(4)		2.4893		2.8931		3.2981	
Injection: (1)		172000		209970		223910	
[Peak Area] (2)		181510		210980		222000	
(3)		103300		106080		103230	
(4)		99185		105800		103700	

04-Nov-86

Results Summary (continued)

RUN Number →	Temperature 4		Temperature 5	
	15		7	
REPLICATE →	No. 1	No. 2	No. 1	No. 2
Group No.	21		21	
Component ID	56		56	
Temperature (C)	25.2		30	
Low Vol (ml)	21		21	
High Vol (ml)	201		201	
System Vol (ml)	250		250	
H _v avg: atm-m ³ /m ³	4.1373	1.0E-25	4.8951	1.0E-25
H _v avg: atm-mol/mol	5622.4		6759.1	
H _v avg: atm-m ³ /mol	1.01E-01	1	1.22E-01	1
H _v avg: kPa-m ³ /mol	10.2635		12.3386	
COV, r [std/mean]	1.75		3.86	
COV, both replic.	—		—	
Observation: (1)	4.1419		5.1031	
[atm-m ³ /m ³] (2)	4.2265		4.7861	
(3)	4.0495		4.9993	
(4)	4.1314		4.6919	
Injection: (1)	261770		274740	
[Peak Area] (2)	258960		272320	
(3)	109070		104170	
(4)	108030		107120	

ANALYSIS COMPLETED ...

Temperature Regression Parameters:

OF POINTS = 5

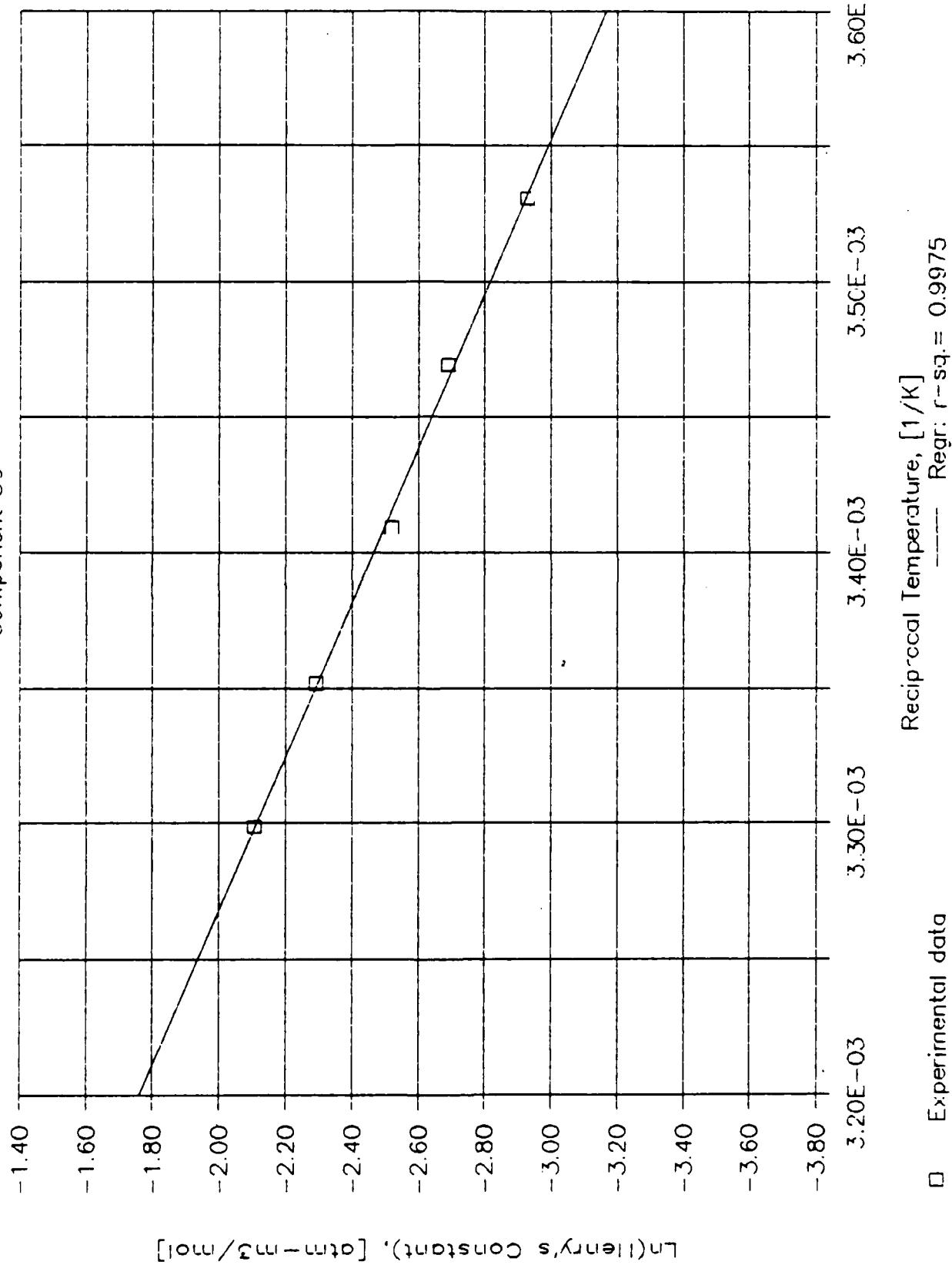
SLOPE = -3.5E+03

Y-INTERCEPT = 9.5E+00

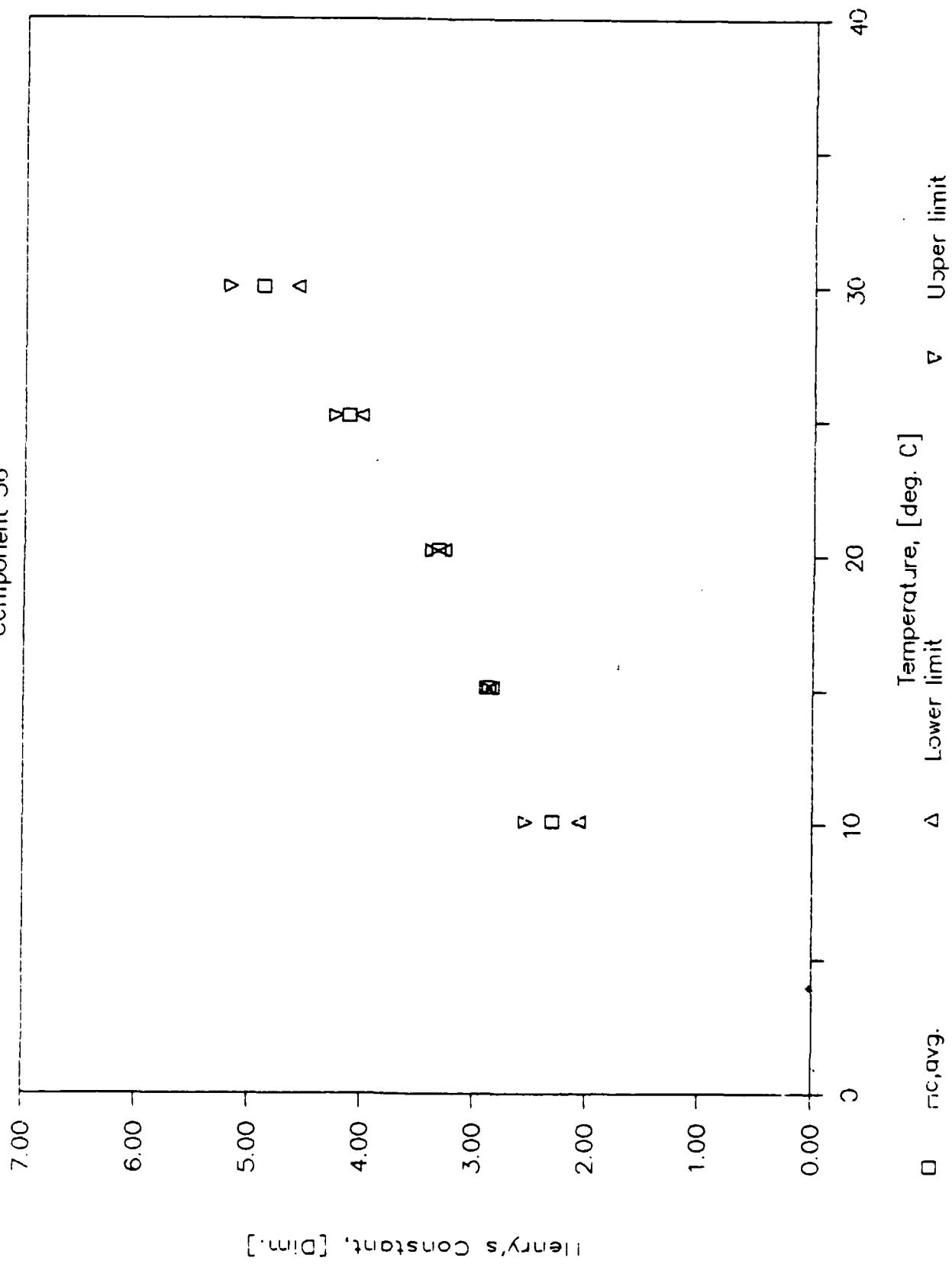
R-SQUARED = 0.9975

TEMPERATURE REGRESSION PLOT
Component 56

362



95% CONFIDENCE TEST
Component 56



REGRESSION CONFIDENCE TEST

Component 56, 95% Confidence

